| Ref # | Hits | Search Query | DBs | Default Operator | Plurals | Time Stamp |
|---|---|---|---|---|---|---|
| L1 | 280 | (514/379).CCLS. | US-PGPUB; USPAT; EPO; DERWENT | OR | OFF | 2005/11/21 10:07 |
| L2 | 387 | (548/241).CCLS. | US-PGPUB; USPAT; EPO; DERWENT | OR | OFF | 2005/11/21 10:07 |

```
Connecting via Winsock to STN


Welcome to STN International!  Enter x:x

LOGINID:SSSPTA1600RXA

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  JUL 20   Powerful new interactive analysis and visualization software,
                   STN AnaVist, now available
 NEWS  4  AUG 11   STN AnaVist workshops to be held in North America
 NEWS  5  AUG 30   CA/CAplus -Increased access to 19th century research documents
 NEWS  6  AUG 30   CASREACT - Enhanced with displayable reaction conditions
 NEWS  7  SEP 09   ACD predicted properties enhanced in REGISTRY/ZREGISTRY
 NEWS  8  OCT 03   MATHDI removed from STN
 NEWS  9  OCT 04   CA/CAplus-Canadian Intellectual Property Office (CIPO) added
                   to core patent offices
 NEWS 10  OCT 06   STN AnaVist workshops to be held in North America
 NEWS 11  OCT 13   New CAS Information Use Policies Effective October 17, 2005
 NEWS 12  OCT 17   STN(R) AnaVist(TM), Version 1.01, allows the export/download
                   of CAplus documents for use in third-party analysis and
                   visualization tools
 NEWS 13  OCT 27   Free KWIC format extended in full-text databases
 NEWS 14  OCT 27   DIOGENES content streamlined
 NEWS 15  OCT 27   EPFULL enhanced with additional content
 NEWS 16  NOV 14   CA/CAplus - Expanded coverage of German academic research

 NEWS EXPRESS  NOVEMBER 18 CURRENT VERSION FOR WINDOWS IS V8.01,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005.
               V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
               http://download.cas.org/express/v8.0-Discover/

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 06:10:29 ON 21 NOV 2005

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
```

FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 06:11:02 ON 21 NOV 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 20 NOV 2005 HIGHEST RN 868524-25-8
DICTIONARY FILE UPDATES: 20 NOV 2005 HIGHEST RN 868524-25-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

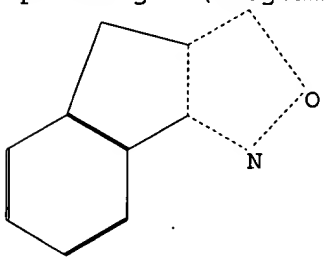
```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
```

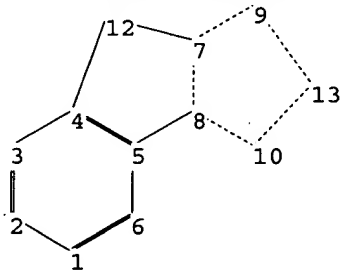
Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\099363561.str



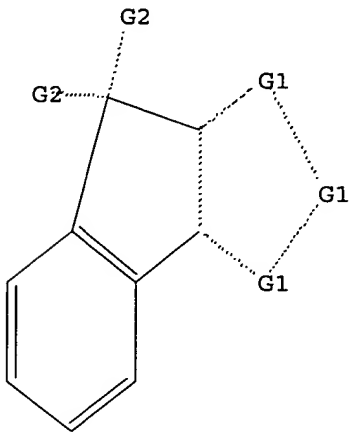

ring nodes :
1 2 3 4 5 6 7 8 9 10 12 13
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-12 5-6 5-8 7-9 7-8 7-12 8-10 9-13 10-13
exact/norm bonds :
4-12 5-8 7-9 7-8 7-12 8-10 9-13 10-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:Atom 13:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR




G1 C,O,N
G2 C,H,O

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 06:11:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 135239 TO ITERATE

1.5% PROCESSED 2000 ITERATIONS 9 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 2683072 TO 2726488
PROJECTED ANSWERS: 10691 TO 13651

L2 9 SEA SSS SAM L1

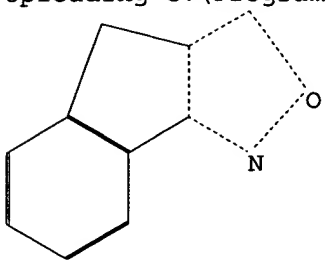
=> s l1 full
FULL SEARCH INITIATED 06:11:22 FILE 'REGISTRY'
<------User Break------>

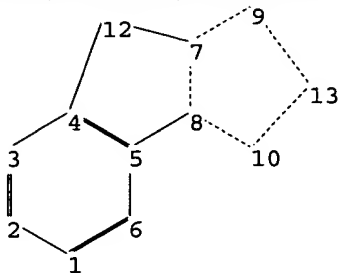
2.2% PROCESSED 60472 ITERATIONS 114 ANSWERS
SEARCH ENDED BY USER
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 2710188 TO 2710188
PROJECTED ANSWERS: 4895 TO 5323

L3 114 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\099363561.str



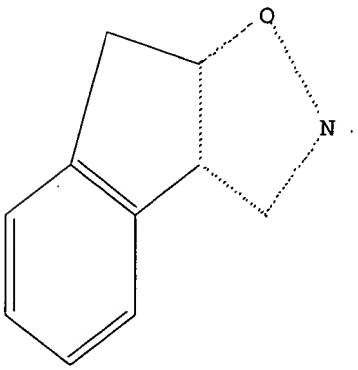




ring nodes :
1 2 3 4 5 6 7 8 9 10 12 13
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-12 5-6 5-8 7-9 7-8 7-12 8-10 9-13 10-13
exact/norm bonds :
4-12 5-8 7-9 7-8 7-12 8-10 9-13 10-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:Atom 13:Atom

L4 STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4 STR

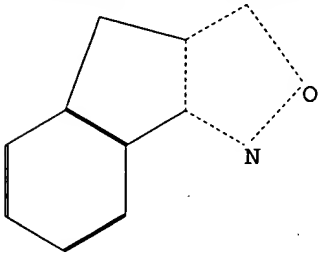


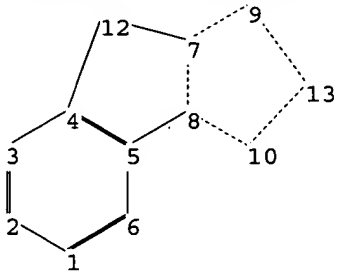

Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 06:12:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 223 TO ITERATE

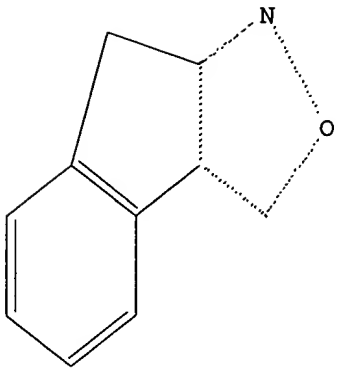
100.0% PROCESSED 223 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          3565 TO     5355
PROJECTED ANSWERS:                2 TO      124

L5             2 SEA SSS SAM L4

=> s l4 full
FULL SEARCH INITIATED 06:12:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     4164 TO ITERATE

100.0% PROCESSED     4164 ITERATIONS                                  27 ANSWERS
SEARCH TIME: 00.00.02

L6             27 SEA SSS FUL L4

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\099363561.str
```



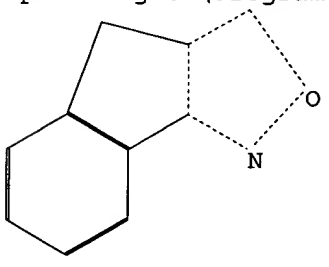



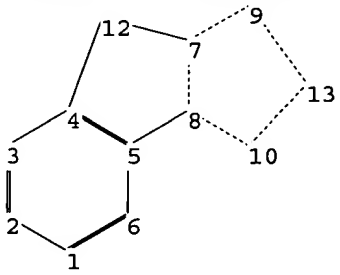

```
ring nodes :
1  2  3  4  5  6  7  8  9  10  12  13
ring bonds :
1-2  1-6  2-3  3-4  4-5  4-12  5-6  5-8  7-9  7-8  7-12  8-10  9-13  10-13
exact/norm bonds :
4-12  5-8  7-9  7-8  7-12  8-10  9-13  10-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
12:Atom  13:Atom



L7      STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7              STR
```




Structure attributes must be viewed using STN Express query preparation.

```
=> s l7
SAMPLE SEARCH INITIATED 06:12:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      283 TO ITERATE

100.0% PROCESSED      283 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         4651 TO     6669
PROJECTED ANSWERS:               0 TO        0

L8             0 SEA SSS SAM L7

=> s l7 full
FULL SEARCH INITIATED 06:12:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     5677 TO ITERATE

100.0% PROCESSED     5677 ITERATIONS                                  4 ANSWERS
SEARCH TIME: 00.00.01

L9             4 SEA SSS FUL L7

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\099363561.str
```



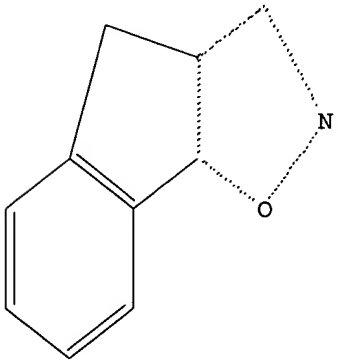

```
ring nodes :
1  2  3  4  5  6  7  8  9  10  12  13
ring bonds :
1-2  1-6  2-3  3-4  4-5  4-12  5-6  5-8  7-9  7-8  7-12  8-10  9-13  10-13
exact/norm bonds :
4-12  5-8  7-9  7-8  7-12  8-10  9-13  10-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
```

containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:Atom 13:Atom

L10 STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10 STR




Structure attributes must be viewed using STN Express query preparation.

=> s l10
SAMPLE SEARCH INITIATED 06:13:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 223 TO ITERATE

100.0% PROCESSED 223 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.06

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3565 TO 5355
PROJECTED ANSWERS: 5 TO 234

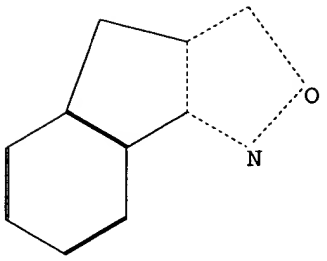
L11 5 SEA SSS SAM L10

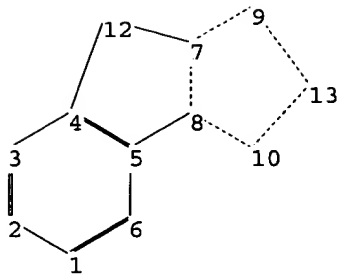
=> s l10 ful
FULL SEARCH INITIATED 06:14:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4164 TO ITERATE

100.0% PROCESSED 4164 ITERATIONS 75 ANSWERS
SEARCH TIME: 00.00.01

L12 75 SEA SSS FUL L10

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\099363561.str



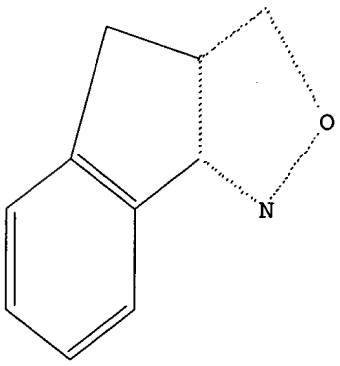




ring nodes :
1 2 3 4 5 6 7 8 9 10 12 13
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-12 5-6 5-8 7-9 7-8 7-12 8-10 9-13 10-13
exact/norm bonds :
4-12 5-8 7-9 7-8 7-12 8-10 9-13 10-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:Atom 13:Atom

L13 STRUCTURE UPLOADED

=> d
L13 HAS NO ANSWERS
L13 STR




Structure attributes must be viewed using STN Express query preparation.

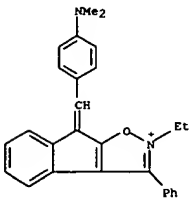
=> s l13
SAMPLE SEARCH INITIATED 06:14:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 283 TO ITERATE

100.0% PROCESSED 283 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

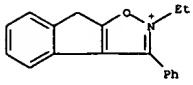
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4651 TO 6669

```
PROJECTED ANSWERS:                1 TO       80

L14            1 SEA SSS SAM L13

=> s l13 full
FULL SEARCH INITIATED 06:14:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      5677 TO ITERATE

100.0% PROCESSED     5677 ITERATIONS                                  13 ANSWERS
SEARCH TIME: 00.00.03

L15           13 SEA SSS FUL L13

=> s l6 and caplus/lc
      48972147 CAPLUS/LC
L16          24 L6 AND CAPLUS/LC

=> s l6 not l16
L17           3 L6 NOT L16

=> d 1-3
```

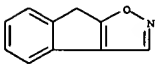
L17 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN 47649-55-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 8H-Indeno[1,2-d]isoxazolium, 8-[[4-(dimethylamino)phenyl]methylene]-2-ethyl-3-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H25 N2 O
CI COM




L17 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN 47044-14-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN 8H-Indeno[1,2-d]isoxazolium, 2-ethyl-3-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H16 N O
CI COM



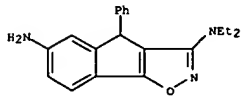

L17 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN 319-10-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 8H-Indeno[1,2-d]isoxazole (8CI, 9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H7 N O




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

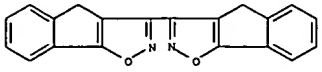
```
=> s l9 and caplus/lc
      48972147 CAPLUS/LC
L18           4 L9 AND CAPLUS/LC

=> s l12 and caplus/lc
      48972147 CAPLUS/LC
L19          70 L12 AND CAPLUS/LC

=> s l12 not l19
L20           5 L12 NOT L19

=> d 1-5
```

L20 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
RN 838884-34-7 REGISTRY
ED Entered STN: 28 Feb 2005
CN INDEX NAME NOT YET ASSIGNED
FS 3D CONCORD
MF C20 H21 N3 O
SR Chemical Library
Supplier: ChemBridge Corporation
LC STN Files: CHEMCATS



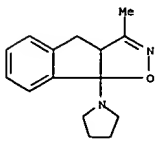
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L20 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
RN 502181-33-1 REGISTRY
ED Entered STN: 08 Apr 2003
CN 3,3'-Bi-4H-indeno[2,1-d]isoxazole (9CI) (CA INDEX NAME)
OTHER NAMES:
CN NSC 371686
FS 3D CONCORD
MF C20 H12 N2 O2
SR Chemical Library



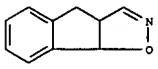
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L20 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
RN 46849-31-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-methyl-8b-(1-pyrrolidinyl)-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H18 N2 O
CI COM
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)



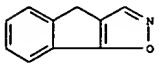
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L20 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
RN 5695-19-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro- (8CI) (CA INDEX NAME)
OTHER NAMES:
CN 3a,8b-Dihydro-4H-indeno[2,1-d]isoxazole
CN 4,5-(2,1-Indano)-2-isoxazoline
FS 3D CONCORD
MF C10 H9 N O



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L20 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
RN 247-33-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN 4H-Indeno[2,1-d]isoxazole (8CI, 9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H7 N O




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

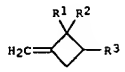
```
=> s l14 and caplus/lc
      48972147 CAPLUS/LC
L21           1 L14 AND CAPLUS/LC

=> s l14 and caplus/lc
      48972147 CAPLUS/LC
L22           1 L14 AND CAPLUS/LC

=> s l14 not l22
L23           0 L14 NOT L22

=> s l15 and caplus/lc
      48972147 CAPLUS/LC
L24          13 L15 AND CAPLUS/LC

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   851.55     851.76

FILE 'CAPLUS' ENTERED AT 06:17:35 ON 21 NOV 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
```



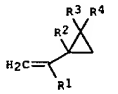
```
FILE COVERS 1907 - 21 Nov 2005  VOL 143 ISS 22
FILE LAST UPDATED: 20 Nov 2005  (20051120/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l16
L25          10 L16

=> d ibib abs hitstr 1-10
```

L25 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

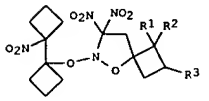
ACCESSION NUMBER: 2004:574043 CAPLUS
DOCUMENT NUMBER: 142:155884
TITLE: Three-component reactions of tetranitromethane with olefins
AUTHOR(S): Averina, E. B.; Budynina, E. M.; Ivanova, O. A.; Grishin, Yu. K.; Gerdov, S. M.; Kuznetsova, T. S.; Zefirov, N. S.
CORPORATE SOURCE: Moscow State University, Moscow, 119899, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2004), 40(2), 162-173
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:155884
GI



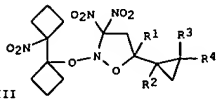
I



II



III



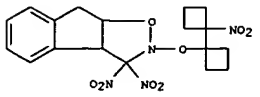
IV

AB Three-component reactions of tetranitromethane with two different olefins,
e.g. cyclobutylenecyclobutane and cyclobutane derivs. (I) (R1 = R2 = R3 = R4 = H; R1 = R2 = CH2CH2, R3 = H; R1 = R2 = H, R3 = cyano) or vinylcyclobutane derivs. (II) (R1' = R2' = R3' = R4' = H; R1' = cyclopropyl, R2' = R3' = R4' = H; R1' = R2' = H, R3' = R4' = CO2Et; R1' = Me, R2' = isopropenyl, R3' = R4' = H), taken in equimolar amts. are procedures fit for preparation of 3,3-dinitroisoxazolidines of a mixed composition,
e.g. (III) or (IV).

IT **828922-53-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dinitroisoxazolidine derivs. by three-component cycloaddn.
reactions of tetranitromethane with olefins)

RN 828922-53-8 CAPLUS
CN 2H-Indeno[1,2-d]isoxazole, 3,3a,8,8a-tetrahydro-3,3-dinitro-2-[(1'-nitro[1,1'-bicyclobutyl]-1-yl)oxy]- (9CI) (CA INDEX NAME)

L25 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

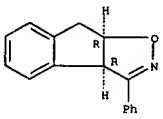
ACCESSION NUMBER: 1998:358689 CAPLUS
DOCUMENT NUMBER: 129:109016
TITLE: One-pot synthesis of isoxazoline derivatives by sonochemical activation
AUTHOR(S): Bougrin, Khalid; Lamiri, Mustapha; Soufiaoui, Mohamed
CORPORATE SOURCE: Laboratoire de Chimie des Plantes et de Synthese Organique et Bioorganique, Universite Mohammed V, Faculte des Sciences, Rabat, 1014 R.P., Morocco
SOURCE: Tetrahedron Letters (1998), 39(25), 4455-4458
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: French

AB Several isoxazolines are prepared from oximes and olefins in the biphasic system Ca(OCl)2/CH2Cl2 or NaOCl/CH2Cl2. Yields are increased under sonication when compared to classical stirring under the same conditions.

IT **210035-72-6P 210035-73-7P 210035-74-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot synthesis of isoxazoline derivs. by sonochem. activation)

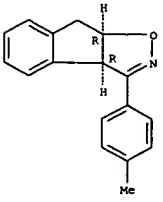
RN 210035-72-6 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-phenyl-, (3aR,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 210035-73-7 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-(4-methylphenyl)-, (3aR,8aR)-rel- (9CI) (CA INDEX NAME)

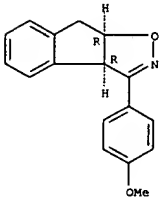
Relative stereochemistry.



RN 210035-74-8 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-(4-methoxyphenyl)-, (3aR,8aR)-rel- (9CI) (CA INDEX NAME)

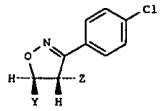
L25 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Relative stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:794721 CAPLUS
DOCUMENT NUMBER: 128:75333
TITLE: 1,3-Dipolar addition of aryl nitrile oxides to some olefinic dipolarophiles in the presence of alumina in dry medium and under microwave irradiation
AUTHOR(S): Syassi, Bouazza; Bougrin, Khalid; Soufiaoui, Mohamed
CORPORATE SOURCE: Lab. Chimie Plantes Synthese Organique Bioorganique, Fac. Scis., Univ. Mohammed V., Rabat, 1014, Morocco
SOURCE: Tetrahedron Letters (1997), 38(51), 8855-8858
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



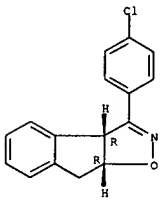
I

AB Isoxazolines, e.g., I (Y = H, Ph, Z = CO2Bu, CO2Et, COPh), are prepared in good yields on solid mineral support in "dry media" and under microwave irradiation in domestic ovens.

IT **200575-68-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(dipolar addition of arylnitrile oxides to olefinic compds. under microwave irradiation to give isoxazolines)

RN 200575-68-4 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3-(4-chlorophenyl)-3a,8a-dihydro-, cis- (9CI) (CA INDEX NAME)

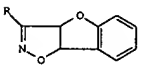
Relative stereochemistry.



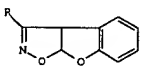
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L25 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:475171 CAPLUS
DOCUMENT NUMBER: 89:75171
TITLE: Selectivity in cycloadditions. 6. Cycloadditions of nitrile oxides to benzofuran. Regiochemistry
AUTHOR(S): Caramella, P.; Cellerino, G.; Houk, K. N.; Albini, F. Marinone; Santiago, Cielo
CORPORATE SOURCE: Dep. Chem., Louisiana State Univ., Baton Rouge, LA, USA
SOURCE: Journal of Organic Chemistry (1978), 43(15), 3006-10
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

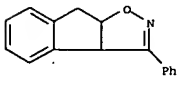


II

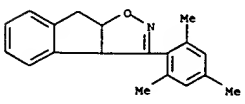
AB Cycloaddn. of RCNO (I; R = Ph, 2,4,6-Me3C6H2) to benzofuran yielded the 2 regioisomeric cycloadducts in 70:30 and 26:74 ratio, resp. Frontier-orbital considerations, using ab initio STO-3G, CNDO/2 or EHMO calcns., and a comparison with the regioselectivities observed with indene and styrene allowed elucidation of the inversion of regiochem. of the cycloaddns. of I to benzofuran.

IT **42443-92-5P 61191-74-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

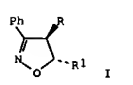
RN 42443-92-5 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



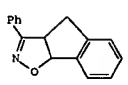
RN 61191-74-0 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



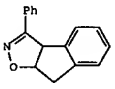
L25 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:4459 CAPLUS
DOCUMENT NUMBER: 86:4459
TITLE: Δ2-Isoxazoline derivatives. Part X. 1,3-Dipolar cycloadditions of nitrones and nitrile oxides with indene, 1,2-dihydrodnaphthalene, and trans-1-phenylpropene
AUTHOR(S): Bianchi, Giorgio; De Micheli, Carlo; Gandolfi, Remo
CORPORATE SOURCE: Ist. Chim. Org., Univ. Pavia, Pavia, Italy
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (14), 1518-23
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

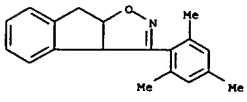


III

AB Reaction of cyclic and acyclic nitrones and nitrile oxides with 1,2-dihydronaphthalene, indene, and trans-MeCH:CHPh gave mixts. of regioisomers. E.g., PhC.tplbond.NO with trans-MeCH:CHPh gave 43.5% of a 66:34 mixture of isoxazolines I (R = Me, R1 = Ph; R = Ph, R1 = Me) and with indene 91% of a 98:2 mixture of II and III was formed. The results are analyzed on the basis of frontier orbital interactions and steric requirements of the reagents; transition state structures for the reactions are proposed.

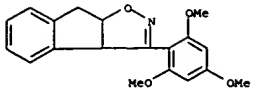
IT **61191-74-0P 61191-76-2P 61191-80-8P 61218-36-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 61191-74-0 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



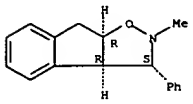
RN 61191-76-2 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-(2,4,6-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L25 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



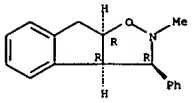
RN 61191-80-8 CAPLUS
CN 2H-Indeno[1,2-d]isoxazole, 3,3a,8,8a-tetrahydro-2-methyl-3-phenyl-, (3α,3aα,8aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

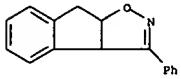


RN 61218-36-8 CAPLUS
CN 2H-Indeno[1,2-d]isoxazole, 3,3a,8,8a-tetrahydro-2-methyl-3-phenyl-, (3α,3aβ,8aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



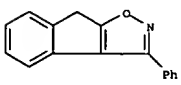
L25 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:465646 CAPLUS
DOCUMENT NUMBER: 79:65646
TITLE: Selectivity in cycloadditions. III. Regioselectivity and π-conjugation in the 1,3-dipolar cycloadditions of benzonitrile oxide
AUTHOR(S): Bailo, Giorgio; Caramella, Pierluigi; Cellerino, Giuseppe; Invernizzi, Anna G.; Gruenanger, Paolo
CORPORATE SOURCE: Ist. Chim. Org., Univ. Pavia, Pavia, Italy
SOURCE: Gazzetta Chimica Italiana (1973), 103(1-2), 47-59
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Treatment of benzohydroxamic acid chloride with Et3N in Et2O at 0° gave PhC.tplbond.NO which cyclo-added to cyclopentadiene to give 94% of a mixture of monoadducts containing 99% I and 1% II. Further cycloaddn. of PhC.tplbond.NO to I give a mixture containing 30% anti-III, 45% anti-IV, 6% syn-III, and 19% syn-IV. Similarly, cycloaddn. to II give a mixture containing 39% anti-IV, 43% anti-V, 18% syn-IV, and 0% syn-V. The cycloaddn. of PhC.tplbond.NO to indene also gave a mixture containing 98% VI and 2% VII. The π-configurative control of the highly regioselective cycloaddn. of PhC.tplbond.NO to cyclopentadiene and indene was contrasted to the lack of regiospecificity or -selectivity in the cycloaddn. of PhC.tplbond.NO to 6,6-dimethyl- and 6,6-diphenylfulvene. The frontier orbital interactions of PhC.tplbond.NO with indene and cyclopentadiene were discussed.
IT **42443-92-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42443-92-5 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



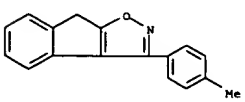
L25 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:112961 CAPLUS
DOCUMENT NUMBER: 76:112961
TITLE: Pharmacologically active 1,2-substituted indene compounds
INVENTOR(S): Trepanier, Donald L.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 3636116 | A | 19720118 | US 1968-757102 | 19680903 |
| US 3719674 | A | 19730306 | US 1971-113744 | 19710208 |
| PRIORITY APPLN. INFO.: | | | US 1968-757102 | A3 19680903 |

GI For diagram(s), see printed CA Issue.
AB Treatment of indene with substituted chlorobenzohydroxamoyl chlorides gave indenoisoxazoles (I, R1, R2, R3 = H, Cl, Br, Me), which were reduced to 2-(α-aminosubstituted benzyl)-1-indanols, which when treated with BrCN and cyclized, gave the indenooxazines (II, R1, R2, R3 = H, Cl, Br, Me). The compds. were amphetamine and barbiturate potentiators. Thus, Et3N was added to CHCl3 containing 4-chloro-benzohydroxamoyl chloride and indene and the mixture refluxed to give I (R1 = R3 = H, R2 = 4-Cl) (III). III was reduced by LiAlH4 in Et2O to give 2-(α-amino-4-chlorobenzyl)-1-indanol, which when administered to mice at 65 mg/kg with hexobarbital, doubled the mice sleep time. Five other I, 3 indanols, 3 BrCN-indanol reaction products, and 4 II were prepared
IT **36288-35-4P 36288-36-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36288-35-4 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3-phenyl- (9CI) (CA INDEX NAME)



RN 36288-36-5 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

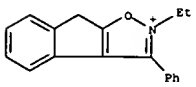


L25 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L25 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:11627 CAPLUS
DOCUMENT NUMBER: 70:11627
TITLE: Pseudoazulenes. VI. Indenopyrazoles and the attempted preparation of an indenoisoxazole
AUTHOR(S): Boyd, Gerhard V.; Hewson, David
CORPORATE SOURCE: Chelsea Coll. Sci. Technol., London, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1968), (23), 2959-64
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:11627
GI For diagram(s), see printed CA Issue.
AB 2-Methyl-1,3-diphenylindeno [2,1-c]pyrazole (I) and the 3-ethoxycarbonyl analog of I, derivs. of a novel pseudoazulenic system containing two fused fived-membered rings were prepared The direction of addition of nitrilimines to indanone-enamines was established. The pseudo-azulenes are protonated on the five-membered carbon ring. Azo-coupling, tropylation, formylation, and condensation with p-Me2NC6H4CHO was carried out on I; the structures of the products and of their conjugate acids are discussed.
IT **21405-92-5P 21405-93-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21405-92-5 CAPLUS
CN 8H-Indeno[1,2-d]isoxazolium, 2-ethyl-3-phenyl-, tetrafluoroborate(1-) (8CI) (CA INDEX NAME)

CM 1

CRN 47044-14-4
CMF C18 H16 N O



CM 2

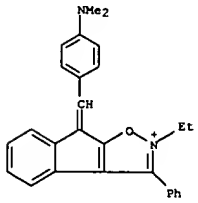
CRN 14874-70-5
CMF B F4
CCI CCS

RN 21405-93-6 CAPLUS

L25 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 8H-Indeno[1,2-d]isoxazolium, 8-[p-(dimethylamino)benzylidene]-2-ethyl-3-phenyl-, tetrafluoroborate(1-) (8CI) (CA INDEX NAME)

CM 1

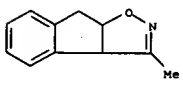
CRN 47649-55-8
CMF C27 H25 N2 O



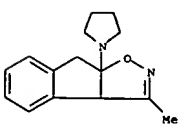
CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

L25 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:500043 CAPLUS
DOCUMENT NUMBER: 67:100043
TITLE: Indenoisoxazole derivatives
AUTHOR(S): Bianchi, Giorgio; Gandolfi, Remo; Gruenanger, Paolo; Perotti, Angelo
CORPORATE SOURCE: Univ. Pavia, Pavia, Italy
SOURCE: Journal of the Chemical Society [Section] C: Organic (1967), (17), 1598-602
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:100043
GI For diagram(s), see printed CA Issue.
AB From the cycloaddn. of acetonitrile N-oxide with indene two isomeric methyldihydroindenoisoxazoles (I and II) were isolated. Elucidation of their structures by bromination and 1H N.M.R. spectroscopy, and related reactions on analogous compds. are described. 17 references.
IT **16565-53-0P 16565-64-3P 16565-65-4P**
**16565-66-5P 16565-67-6P 16565-68-7P**
**16565-69-8P 16614-68-9P 16614-69-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16565-53-0 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-methyl- (8CI) (CA INDEX NAME)



RN 16565-64-3 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-methyl-8a-(1-pyrrolidinyl)- (8CI) (CA INDEX NAME)

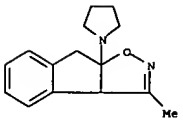


RN 16565-65-4 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-methyl-8a-(1-pyrrolidinyl)-, monomethiodide (8CI) (CA INDEX NAME)

CM 1

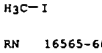
CRN 16565-64-3
CMF C15 H18 N2 O

L25 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

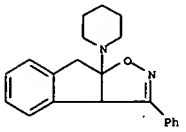


CM 2

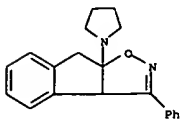
CRN 74-88-4
CMF C H3 I



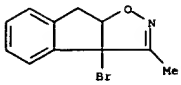
RN 16565-66-5 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-phenyl-8a-piperidino- (8CI) (CA INDEX NAME)



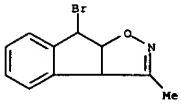
RN 16565-67-6 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-phenyl-8a-(1-pyrrolidinyl)- (8CI) (CA INDEX NAME)



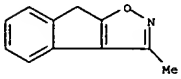
RN 16565-68-7 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a-bromo-3a,8a-dihydro-3-methyl- (8CI) (CA INDEX NAME)



RN 16565-69-8 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 8-bromo-3a,8a-dihydro-3-methyl- (8CI) (CA INDEX NAME)



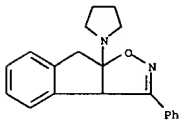
RN 16614-68-9 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3-methyl- (8CI) (CA INDEX NAME)



RN 16614-69-0 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-3-phenyl-8a-(1-pyrrolidinyl)-, monomethiodide (8CI) (CA INDEX NAME)

CM 1

CRN 16565-67-6
CMF C20 H20 N2 O



CM 2

CRN 74-88-4
CMF C H3 I







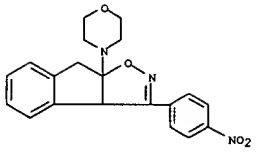
ACCESSION NUMBER: 1964:82853 CAPLUS
DOCUMENT NUMBER: 60:82853
ORIGINAL REFERENCE NO.: 60:14501e-h
TITLE: Enamines. X. Reactions of halohydroxamic acids with enamines of alicyclic compounds
AUTHOR(S): Bianchetti, Giuseppe; Pocar, Donato; Dalla Croce, Piero
CORPORATE SOURCE: Univ. Milan
SOURCE: Gazzetta Chimica Italiana (1963), 93(12), 1726-35
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:82853

AB 1-(N-Morpholinyl)-1-cycloheptene, b13 134°, was prepared by azeotropic removal of H2O from equimolar amts. of cycloheptanone and morpholine in PhMe containing a trace of MeC6H4SO3H, followed by distillation
Similarly was prepared 1-(N-4-methylpiperazinyl)-1-cyclopentene, b0.15 116-18°. Equimolar amts. of II, 1-(N-morpholinyl)-1-cyclohexene, and Et3N boiled in CHCl3 1 hr. and evaporated to an oil that solidified gave V
(R = 4-O2NC6H4, n = 4, R' = N-morpholinyl), m. 138-40° (EtOH). Likewise, by boiling 45 min. to 1 hr. and using the resp. reagents were prepared the following derivs. of V: (R = 4-O2NC6H4, R' = N-morpholinyl, n = 5), m. 180° (MeOH); (R = Ph, R' = N-pyrrolidinyl, n = 4), m. 103°; (R = 4-O2NC6H4, R' = N-morpholinyl, n = 3), m. 154° (EtOH); (R = 4-ClC6H4, R' = N-morpholinyl, n = 3), m. 115° (MeOH); (R = Ph, R' = N-morpholinyl, n = 3), m. 105-6° (ligroine); (R = 4-ClC6H4, R' = N-piperidinyl, n = 3), m. 108° (EtOH); (R = 4-ClC6H4, R' = N-4-methylpiperidinyl, n = 3), m. 120° (ligroine). Also prepared was 3-(4-nitrophenyl)8a-(N-morpholinyl)-3a,8a-dihydroindenol[1,2-d]isoxazole (in absence of Et3N), m. 238° (EtOH). Derivs. of V with n = 4 or 5 were readily hydrolyzed by 10-20% HCl to the corresponding derivs. of VI; thus were prepared: R = 4-O2NC6H4, n = 4, m. 180° (EtOH); R = 4-O2NC6H4, n = 5, m. 132° (MeOH); R = Ph, n = 4, m. 50° (aqueous AcOH); however V with n = 3 were recovered unchanged even with 48% HBr. V (R = Ph, R'' = N-morpholinyl, n = 4), m. 103°, was also prepared as in previous paper from benzonitrile N-oxide and 1-(N-morpholinyl)-1-cyclohexene (VII) in boiling CHCl3, 30 min. VI (R = CO2H, n = 4), m. 128° (H2O), was prepared by boiling 10 g. ClC(:NOH)(CO2Et) and VII in 300 cc. CHCl3 1 hr. and evaporating to an oil
which was extracted with Et2O, filtered, evaporated, and the residue boiled 30 min. with 100 cc. 10% NaOH and then acidified.

IT **90117-24-1**, 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-8a-morpholino-3-(p-nitrophenyl)-
(preparation of)

RN 90117-24-1 CAPLUS
CN 8H-Indeno[1,2-d]isoxazole, 3a,8a-dihydro-8a-morpholino-3-(p-nitrophenyl)-(7CI) (CA INDEX NAME)

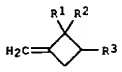




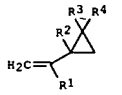
```
=> s l19
L26          37 L19

=> s l26 not l25
L27          30 L26 NOT L25

=> d ibib abs hitstr l26 1-37
```

L26 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

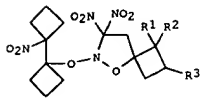
ACCESSION NUMBER: 2004:574043 CAPLUS
DOCUMENT NUMBER: 142:155884
TITLE: Three-component reactions of tetranitromethane with olefins
AUTHOR(S): Averina, E. B.; Budynina, E. M.; Ivanova, O. A.; Grishin, Yu. K.; Gerdov, S. M.; Kuznetsova, T. S.; Zefirov, N. S.
CORPORATE SOURCE: Moscow State University, Moscow, 119899, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2004), 40(2), 162-173
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:155884
GI



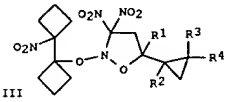
I



II



III



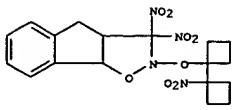
IV

AB Three-component reactions of tetranitromethane with two different olefins,
e.g. cyclobutylenecyclobutane and cyclobutane derivs. (I) (R1 = R2 = R3 = R4 = H; R1 = R2 = CH2CH2, R3 = H; R1 = R2 = H, R3 = cyano) or vinylcyclobutane derivs. (II) (R1' = R2' = R3' = R4' = H; R1' = cyclopropyl, R2' = R3' = R4' = H; R1' = R2' = H, R3' = R4' = CO2Et; R1' = Me, R2' = isopropenyl, R3' = R4' = H), taken in equimolar amts. are procedures fit for preparation of 3,3-dinitroisoxazolidines of a mixed composition,
e.g. (III) or (IV).

IT **828922-54-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dinitroisoxazolidine derivs. by three-component cycloaddn.
reactions of tetranitromethane with olefins)

RN 828922-54-9 CAPLUS
CN 2H-Indeno[2,1-d]isoxazole, 3,3a,4,8b-tetrahydro-3,3-dinitro-2-[(1'-nitro[1,1'-bicyclobutyl]-1-yl)oxy]- (9CI) (CA INDEX NAME)

L26 ANSWER 1 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

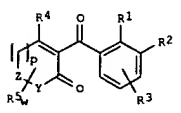
L26 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:171868 CAPLUS
DOCUMENT NUMBER: 136:216742
TITLE: Preparation of 2-[(isoxazol-3-yl)benzoyl]cyclohexane-1,3-diones as herbicides
INVENTOR(S): Van Almsick, Andreas; Willms, Lothar; Auler, Thomas; Bieringer, Hermann; Thuerwaechter, Felix
PATENT ASSIGNEE(S): Aventis CropScience GmbH, Germany
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002018352 | A1 | 20020307 | WO 2001-EP9601 | 20010821 |
| W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CN, CO, CR, CU, CZ, DM, DZ, EC, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PH, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| DE 10043075 | A1 | 20020314 | DE 2000-10043075 | 20000901 |
| AU 2001082108 | A5 | 20020313 | AU 2001-82108 | 20010821 |
| EP 1315706 | A1 | 20030604 | EP 2001-960683 | 20010821 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| US 2002173424 | A1 | 20021121 | US 2001-943040 | 20010830 |
| US 6703348 | B2 | 20040309 | | |

PRIORITY APPLN. INFO.: DE 2000-10043075 A 20000901
WO 2001-EP9601 W 20010821

OTHER SOURCE(S): MARPAT 136:216742
GI



I

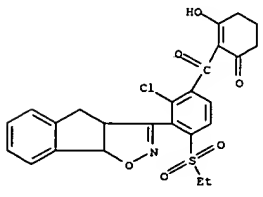
AB Title compds. [I; R1 = halo, (halo)alkyl, alkylsulfenyl, alkylsulfinyl, alkylsulfonyl, NO2; R2 = (substituted) bi-, tri-, or tetracyclic heteroaryl; R3 = halo, haloalkyl, alkylsulfenyl, alkylsulfinyl, alkylsulfonyl, NO2; R4 = OR7, (halo)alkylthio, (halo)alkenylthio, (halo)alkynylthio, (halo)alkylsulfinyl, etc.; R7 = H, (halo)alkyl, alkoxyalkyl, CHO, alkylcarbonyl, etc.; R5 = tetrahydropyran-3-yl, tetrahydropyran-4-yl, tetrahydrothiopyran-3-yl, alkyl, cycloalkyl, etc.; Y

L26 ANSWER 2 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

= O, S, NH, N-alkyl, CHR5, CR52; Z = O, S, SO, SO2, NH, N-alkyl, CHR5, CR52; p = 0, 1; w = 0-4], were prepd. Thus, 2-chloro-4-methylsulfonyl-3-(3a,4,5,6a-tetrahydrofuro[3,2-d]isoxazol-3-yl)benzoic acid (prepn. given) in CH2Cl2 was treated with (COCl)2 and DMF at room temp. followed by reflux for 1 h and dropwise addn. of 1,3-cyclohexanedione and Et3N in CH2Cl2 to give after 2 h stirring 87% 2-chloro-4-methylsulfonyl-3-(3a,4,5,6a-tetrahydrofuro[3,2-d]isoxazol-3-yl)benzoic acid 3-oxocyclohex-1-enyl ester. The resulting intermediate in MeCN was stirred with Et3N and acetone cyanohydrin for 16 h at room temp. to give 73% 2-[2-chloro-4-methylsulfonyl-3-(3a,4,5,6a-tetrahydrofuro[3,2-d]isoxazol-3-yl)benzoyl]cyclohexane-1,3-dione. The latter at 38-150 ppm postemergent gave 85-95% control of Setaria faberii and 70-90% control of Setaria virdis. The title compds. are esp. useful to combat of Setaria spp. on corn cultures.

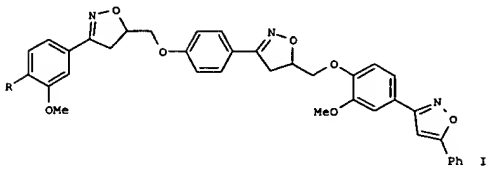
IT **402478-57-3P**
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of (isoxazolylbenzoyl)cyclohexanediones as herbicides)

RN 402478-57-3 CAPLUS
CN 2-Cyclohexen-1-one,
2-[2-chloro-3-(3a,8b-dihydro-4H-indeno[2,1-d]isoxazol-3-yl)-4-(ethylsulfonyl)benzoyl]-3-hydroxy- (9CI) (CA INDEX NAME)

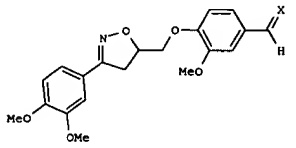


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L26 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:557689 CAPLUS
DOCUMENT NUMBER: 135:344409
TITLE: Synthesis of novel polyheterocyclic compounds
AUTHOR(S): Hassikou, A.; Benabdallah, G. A.; Dinia, M. N.; Bougrin, K.; Soufiaoui, M.
CORPORATE SOURCE: Laboratoire de Chimie des Plantes et de Synthese Organique et Bio-organique, Universite Mohammed V-Agdal, Faculte des Sciences, RP Rabat, Morocco
SOURCE: Tetrahedron Letters (2001), 42(34), 5857-5861
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 135:344409
GI



I

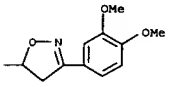


II

AB New polyheterocyclic compds. containing two or three oxazole or oxazoline moieties such as I (R = MeO) are prepared Alkynyloxy and allyloxybenzaldehydes are prepared; cycloaddn. of nitrile oxides generated in situ from benzaldehyde oximes to the allyl- and propargyloxy moieties gave isooxazolines and isoxazoles with free aldehyde moieties. The aldehyde moieties formed oximes on treatment with hydroxylamine hydrochloride; oxidation of the oximes gave nitrile oxides in situ which reacted with di-Me acetylenedicarboxylate, phenylacetylene, indene, and an allyloxybenzaldehyde to give isoxazoles and isoxazolines. E.g., treatment

L26 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 1-B



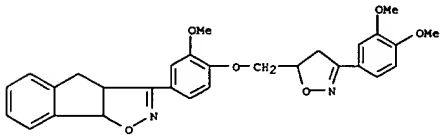
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 3 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

of 3-hydroxy-4-methoxybenzaldehyde with propargyl bromide gave 3-methoxy-4-(propargyloxy)benzaldehyde; cycloaddn. with 3,4-dimethoxybenzaldehyde oxime in the presence of sodium hypochlorite in methylene chloride and water gave a phenylisoxazolylmethoxybenzaldehyde II (X = O) in 75% yield. E.g., treatment of II (X = O) with hydroxylamine hydrochloride and sodium hydroxide gave oxime II [R = (HO)N]; oxidn. of II [X = (HO)N] and addn. of an allyloxybenzaldehyde gave an aldehyde contg. isoxazole and isoxazolidine moieties; treatment of the aldehyde with hydroxylamine hydrochloride, oxidn. and treatment with phenylacetylene gave I.

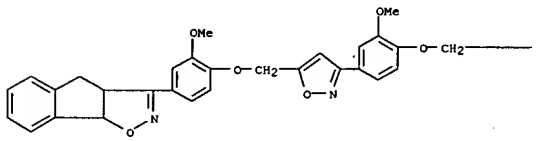
IT **370865-91-1P 370865-94-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of compds. with multiple isoxazole or isoxazoline moieties)

RN 370865-91-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-[4-[[3-(3,4-dimethoxyphenyl)-4,5-dihydro-5-isoxazolyl]methoxy]-3-methoxyphenyl]-3a,8b-dihydro- (9CI) (CA INDEX NAME)

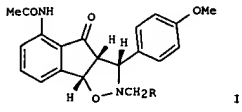


RN 370865-94-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-[4-[[3-[4-[[3-(3,4-dimethoxyphenyl)-4,5-dihydro-5-isoxazolyl]methoxy]-3-methoxyphenyl]-5-isoxazolyl]methoxy]-3-methoxyphenyl]-3a,8b-dihydro- (9CI) (CA INDEX NAME)

PAGE 1-A



L26 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:330717 CAPLUS
DOCUMENT NUMBER: 135:137419
TITLE: Lanthanide triflate catalyzed 1,3-dipolar cycloaddition reactions: stereoselective synthesis of indenoisoxazolidines
AUTHOR(S): Nugiel, D. A.
CORPORATE SOURCE: DuPont Pharmaceuticals, Wilmington, DE, 19880-0336, USA
SOURCE: Tetrahedron Letters (2001), 42(21), 3545-3547
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:137419
GI



I

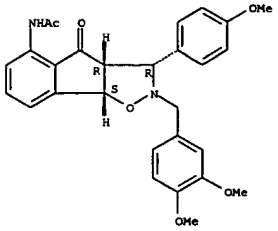
AB Substituted indenones reacted smoothly with a variety of in situ generated nitrones in the presence of lanthanide triflates to give exclusive exo 1,3-dipolar cycloaddn. products, I (R = Ph, 4-MeOC6H4, 3,4-(MeO)2C6H3) in high yield. Judicious choice of the nitrone substituents allowed for further modification of the indenoisoxazolidine core to the corresponding indenoisoxazoline and indenoisoxazole analogs in high yield.

IT **352000-71-6P 352000-76-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(lanthanide triflate catalyzed 1,3-dipolar cycloaddn. reactions, stereoselective synthesis of indenoisoxazolidines)

RN 352000-71-6 CAPLUS
CN Acetamide, N-[(3R,3aR,8bS)-2-[(3,4-dimethoxyphenyl)methyl]-3,3a,4,8b-tetrahydro-3-(4-methoxyphenyl)-4-oxo-2H-indeno[2,1-d]isoxazol-5-yl]-, rel-
(9CI) (CA INDEX NAME)

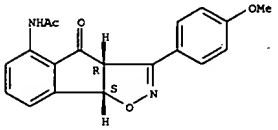
Relative stereochemistry.

L26 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



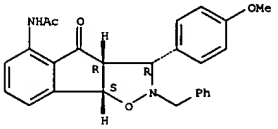
RN 352000-76-1 CAPLUS
CN Acetamide, N-[(3aR,8bS)-3a,8b-dihydro-3-(4-methoxyphenyl)-4-oxo-4H-indeno[2,1-d]isoxazol-5-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

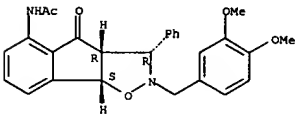


IT **352000-69-2P 352000-70-5P 352000-72-7P**
**352000-73-8P 352000-75-0P 352000-77-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(lanthanide triflate catalyzed 1,3-dipolar cycloaddn. reactions, stereoselective synthesis of indenoisoxazolidines)
RN 352000-69-2 CAPLUS
CN Acetamide,
N-[(3R,3aR,8bS)-3,3a,4,8b-tetrahydro-3-(4-methoxyphenyl)-4-oxo-2-(phenylmethyl)-2H-indeno[2,1-d]isoxazol-5-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

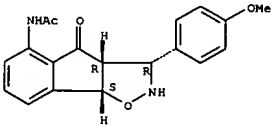


L26 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

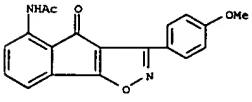


RN 352000-75-0 CAPLUS
CN Acetamide,
N-[(3R,3aR,8bS)-3,3a,4,8b-tetrahydro-3-(4-methoxyphenyl)-4-oxo-2H-indeno[2,1-d]isoxazol-5-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



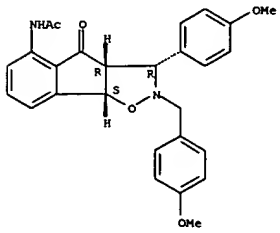
RN 352000-77-2 CAPLUS
CN Acetamide, N-[3-(4-methoxyphenyl)-4-oxo-4H-indeno[2,1-d]isoxazol-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

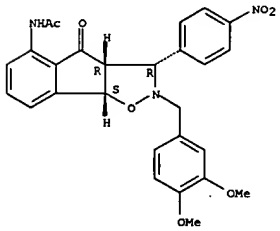
L26 ANSWER 4 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 352000-70-5 CAPLUS
CN Acetamide,
N-[(3R,3aR,8bS)-3,3a,4,8b-tetrahydro-3-(4-methoxyphenyl)-2-[(4-methoxyphenyl)methyl]-4-oxo-2H-indeno[2,1-d]isoxazol-5-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 352000-72-7 CAPLUS
CN Acetamide, N-[(3R,3aR,8bS)-2-[(3,4-dimethoxyphenyl)methyl]-3,3a,4,8b-tetrahydro-3-(4-nitrophenyl)-4-oxo-2H-indeno[2,1-d]isoxazol-5-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

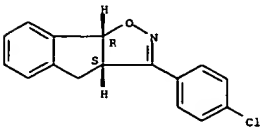


RN 352000-73-8 CAPLUS
CN Acetamide, N-[(3R,3aR,8bS)-2-[(3,4-dimethoxyphenyl)methyl]-3,3a,4,8b-tetrahydro-4-oxo-3-phenyl-2H-indeno[2,1-d]isoxazol-5-yl]-, rel- (9CI) (CA
INDEX NAME)

Relative stereochemistry.

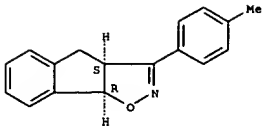
L26 ANSWER 5 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:621500 CAPLUS
DOCUMENT NUMBER: 131:351263
TITLE: New method for synthesis of 4,5-dihydroisoxazoles in solid-liquid biphase media and by ultrasonic activation
AUTHOR(S): Syassi, Bouazza; El Bakkali, Bouchra; Benabdellah, Ghita Amine; Hassikou, Amina; Dinia, Mohamed Nacer; Riviere, Monique; Bougrin, Khalid; Soufiaoui, Mohamed
CORPORATE SOURCE: Laboratoire de Chimie des Plantes et de Synthese Organique et Bioorganique, Universite Mohammed V, Rabat, B.P. 1014 R.P., Morocco
SOURCE: Tetrahedron Letters (1999), 40(40), 7205-7209
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: French
AB A novel methodol. is developed for a one-pot synthesis of 4,5-dihydroisoxazoles. 1-Sodio-3,5-dichloro-s-triazine-2,4,6-trione, alumina, dichloromethane, arylaldoximes, dipolarophiles and ultrasound irradiation are the leading ingredients in the success of this selective reaction. All heterocycles are obtained with good yields and high purity by comparison with classical stirring in the same conditions.
IT **200575-65-1P 250362-70-0P 250362-71-1P**
**250362-72-2P 250362-73-3P 250362-74-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dihydroisoxazoles in solid-liquid biphase media and under
ultrasonic activation)
RN 200575-65-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(4-chlorophenyl)-3a,8b-dihydro-, (3aR,8bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



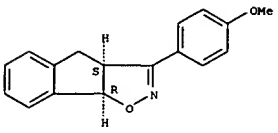
RN 250362-70-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(4-methylphenyl)-, (3aR,8bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



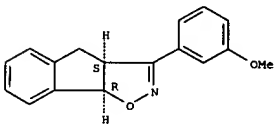
RN 250362-71-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(4-methoxyphenyl)-, (3aR,8bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 250362-72-2 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(3-methoxyphenyl)-, (3aR,8bS)-rel- (9CI) (CA INDEX NAME)

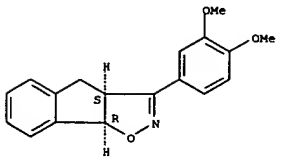
Relative stereochemistry.



RN 250362-73-3 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(3,4-dimethoxyphenyl)-3a,8b-dihydro-, (3aR,8bS)-rel- (9CI) (CA INDEX NAME)

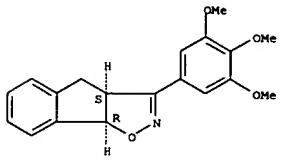
Relative stereochemistry.





RN 250362-74-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(3,4,5-trimethoxyphenyl)-, (3aR,8bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

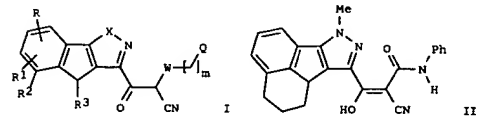


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT


ACCESSION NUMBER: 1999:113652 CAPLUS
DOCUMENT NUMBER: 130:182459
TITLE: Preparation of condensed pyrazole compounds as a kynurenine-3-hydroxylase inhibitors
INVENTOR(S): Varasi, Mario; Pevarello, Paolo; Heidempergher, Franco; Toma, Salvatore; Speciale, Carmela
PATENT ASSIGNEE(S): Pharmacia & Upjohn S.p.A., Italy
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

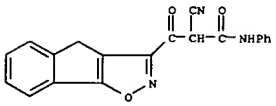
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9906374 | A1 | 19990211 | WO 1998-EP4217 | 19980702 |
| W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KE, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| CA 2297096 | AA | 19990211 | CA 1998-2297096 | 19980702 |
| AU 9888066 | A1 | 19990222 | AU 1998-88066 | 19980702 |
| EP 1001940 | A1 | 20000524 | EP 1998-939623 | 19980702 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| JP 2001512106 | T2 | 20010821 | JP 2000-505133 | 19980702 |
| PRIORITY APPLN. INFO.: | | | GB 1997-16103 A | 19970730 |
| | | | WO 1998-EP4217 W | 19980702 |

OTHER SOURCE(S): MARPAT 130:182459
GI

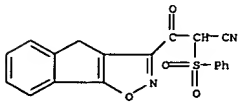


AB The title compds. {I; W = CONH, SO2, CO; X = O, NR4 (wherein R4 = H, C1-6 alkyl, PhCH2, etc.); R, R1, R2 = H, halo, OH, etc.; R3 = H; R2R3 taken together = C2-6 alkylene, CH:CHCH:, O(CH2)n chain in which n = 1-3; m = 0-6; Q = C1-14 alkyl, (un)substituted Ph ring or an unsatd. pentat. heteromonocyclic ring containing two or three heteroatoms which are the same or different and are chosen independently from O, S and N], useful as a kynurenine-3-hydroxylase inhibitors, were prepared and formulated. Thus, treatment of 2-cyano-N-phenyl-3-(7-methyl-2,3,7,9b-tetrahydro-1H-

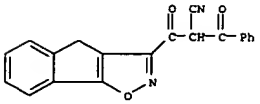

acenaphthol[1,2-c]pyrazol-9-yl)-3-oxopropionamide (prepn. given) with 0.1 N NaOH in EtOH afforded acrylamide II as its sodium salt which showed IC50 of 0.14 μM against KYN-3-OH.
IT **220504-21-2P 220504-22-3P 220504-23-4P 220504-36-9P 220504-37-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of condensed pyrazole compds. as a kynurenine-3-hydroxylase inhibitors)
RN 220504-21-2 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-propanamide, α-cyano-β-oxo-N-phenyl- (9CI) (CA INDEX NAME)



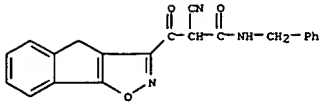
RN 220504-22-3 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-propanenitrile, β-oxo-α-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



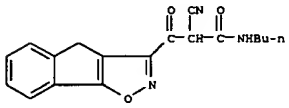
RN 220504-23-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-propanenitrile, α-benzoyl-β-oxo- (9CI) (CA INDEX NAME)



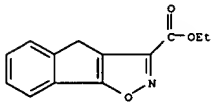
RN 220504-36-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-propanamide, α-cyano-β-oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



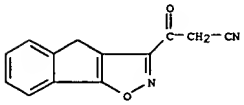
RN 220504-37-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-propanamide, N-butyl-α-cyano-β-oxo- (9CI) (CA INDEX NAME)



IT **220504-38-1P 220504-39-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of condensed pyrazole compds. as a kynurenine-3-hydroxylase inhibitors)
RN 220504-38-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-carboxylic acid, ethyl ester (9CI) (CA INDEX NAME)



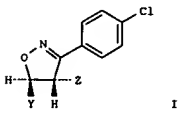
RN 220504-39-2 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-propanenitrile, β-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT



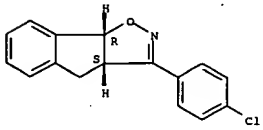
L26 ANSWER 7 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:794721 CAPLUS
DOCUMENT NUMBER: 128:75333
TITLE: 1,3-Dipolar addition of aryl nitrile oxides to some olefinic dipolarophiles in the presence of alumina in dry medium and under microwave irradiation
AUTHOR(S): Syassi, Bouazza; Bougrin, Khalid; Soufiaoui, Mohamed
CORPORATE SOURCE: Lab. Chimie Plantes Synthese Organique Bioorganique, Fac. Scis., Univ. Mohammed V., Rabat, 1014, Morocco
SOURCE: Tetrahedron Letters (1997), 38(51), 8855-8858
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

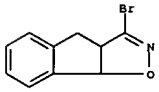
AB Isoxazolines, e.g., I (Y = H, Ph, Z = CO2Bu, CO2Et, COPh), are prepared in good yields on solid mineral support in "dry media" and under microwave irradiation in domestic ovens.
IT **200575-65-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(dipolar addition of arylnitrile oxides to olefinic compds. under microwave irradiation to give isoxazolines)
RN 200575-65-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(4-chlorophenyl)-3a,8b-dihydro-, (3aR,8bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

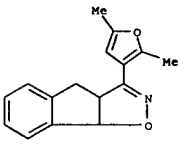
L26 ANSWER 8 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:482236 CAPLUS
DOCUMENT NUMBER: 121:82236
TITLE: A new method for the preparation of β-hydroxy nitriles; transformation of 3-bromo-2-isoxazolines to β-hydroxy nitriles by treatment of alkanethiolates
AUTHOR(S): Seo, Min Hyo; Lee, Youn Young; Goo, Yang Mo
CORPORATE SOURCE: Dep. Chem., Seoul Natl., Seoul, 151-742, S. Korea
SOURCE: Synthetic Communications (1994), 24(10), 1433-9
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:82236
AB 3-Bromo-2-isoxazolines are transformed to β-hydroxy nitriles in good yields by treatment with alkanethiolates under a very mild condition.
IT **156458-62-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring cleavage of, by sodium alkanethiolates, mechanism of β-hydroxy nitriles by)
RN 156458-62-7 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-bromo-3a,8b-dihydro- (9CI) (CA INDEX NAME)



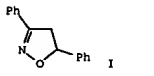
L26 ANSWER 9 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:559011 CAPLUS
DOCUMENT NUMBER: 115:159011
TITLE: 1,3-Dipolar cycloadditions of heterocycles. XXI. Cycloaddition of 2,5-dimethyl-3-furonitrile oxide with cyclic and heterocyclic compounds
AUTHOR(S): Jedlovska, E.; Fisera, L.
CORPORATE SOURCE: Fac. Chem. Technol., Slovak Tech. Univ., Bratislava, CS-812 37, Czech.
SOURCE: Chemical Papers (1991), 45(3), 419-26
CODEN: CHPAEG; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:159011
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

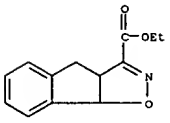
AB Cycloaddns. of 2,5-dimethyl-3-furonitrile oxide (I) to 1,3-cyclohexadiene, 1,3-cyclooctadiene, indene, acenaphthylene, 2,5-dihydrofuran, 2H,4H,7H-1,3-dioxepine, 1,4-epoxy-1,4-dihydronaphthalene, di-Me 7-oxabicyclo[2,2,1]hept-2-ene-5,6-dicarboxylate, di-Me 7-(diphenylmethylene)bicyclo[2,2,1]hept-2-ene-5,6-dicarboxylate, and di-Me 7-oxabicyclo[2,2,1]hept-2,3-diene-2,3-dicarboxylate, are described. Regio- as well as endo/exo selectivity of the reactions, giving adducts II-IV, is discussed. The formation of 1,3-addition products in cycloaddns. to conjugated dienes was not observed
IT **136209-89-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective preparation of, via dipolar cycloaddn. of dimethylfuronitrile oxide)
RN 136209-89-7 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(2,5-dimethyl-3-furanyl)-3a,8b-dihydro- (9CI)
(CA INDEX NAME)



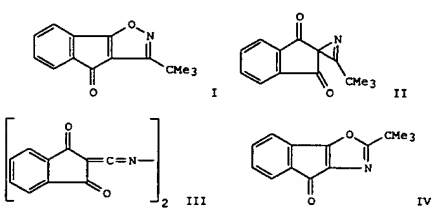
L26 ANSWER 10 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:437762 CAPLUS
DOCUMENT NUMBER: 109:37762
TITLE: New aspects in the hydrogenolytic opening of 2-isoxazolines
AUTHOR(S): Auricchio, Sergio; Ricca, Aldo
CORPORATE SOURCE: Dip. Chim., Politec. Milano, Milan, 20133, Italy
SOURCE: Tetrahedron (1987), 43(17), 3983-6
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:37762
GI



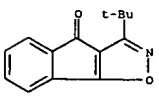
AB The regiochem. of the hydrogenolysis of 2-isoxazolines depends on the substituents present in positions 3 and 5. The hydrogenolysis on 10% Pd-C of 2-isoxazolines, substituted in position 3 with carbonyl or carboxyl groups and in position 5 with an aromatic group, gives oximes, in contrast to other isoxazoline derivs. From the 5-aryl-2-isoxazolines it is possible to obtain aminoalcs. in EtOH and oximes in AcOH. Thus diphenylisoxazole I was hydrogenated in EtOH to quant. give H2NCHPhCH2CH(OH)Ph, whereas in AcOH HON:CPhCH2CH2Ph was obtained.
IT **115106-28-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 115106-28-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole-3-carboxylic acid, 3a,8b-dihydro-, ethyl ester (9CI) (CA INDEX NAME)



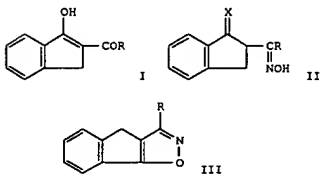
L26 ANSWER 11 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:55779 CAPLUS
DOCUMENT NUMBER: 108:55779
TITLE: Flash vacuum pyrolysis of 3-tert-butylindeno[1,2-c]isoxazol-4-one. Formation of 2-carbonyl-1,3-indandione 2-azine
AUTHOR(S): Perez, Jorge D.; Wunderlin, Daniel A.; Lemke, Thomas L.; Sawhney, Kailash N.
CORPORATE SOURCE: Inst. Invest. Fis. Quim., Fac. Cienc. Quim., Cordoba, 5.016, Argent.
SOURCE: Journal of Heterocyclic Chemistry (1987), 24(4), 1073-6
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:55779
GI



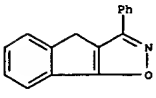
AB Flash vacuum pyrolysis (FVP) of the title isoxazolone (I) at 400° gave 35% azirene II and 65% azine III. At 500°, 70% III and 30% oxazolone IV were obtained. Similarly, FVP of II at 400° gave 17% III and 83% IV.
IT **82501-33-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(flash vacuum pyrolysis of)
RN 82501-33-5 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



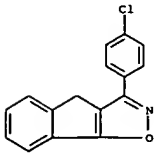
L26 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1986:571931 CAPLUS
DOCUMENT NUMBER: 105:171931
TITLE: Synthesis of novel indene derivatives
AUTHOR(S): Samula, Kazimierz; Cichy, Bozenna
CORPORATE SOURCE: Inst. Pharm. Ind., Warsaw, 01-793, Pol.
SOURCE: Acta Poloniae Pharmaceutica (1985), 42(3), 256-62
CODEN: APPHAX; ISSN: 0001-6837
DOCUMENT TYPE: Journal
LANGUAGE: Polish
OTHER SOURCE(S): CASREACT 105:171931
GI



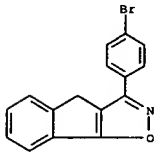
AB The indene derivs. I [R = 4-ClC6H4; 2-, 3-, and 4-pyridyl; 2,4-HO(MeO)C6H3; 2,4-(MeO)2C6H3; 2-thienyl] were prepared in 54-65% yields by the reaction of phthalaldehyde with RCOMe in 15% aqueous NaOH. I, refluxed with NH2OH·HCl in MeOH containing C5H5N, gave 55-81% II [R = 4-ClC6H4, 4-BrC6H4, 3- and 4-pyridyl, Ph, 2-HOC6H4, 2,4-HO(MeO)C6H3; X = O]. In a similar reaction using EtOH and morpholine, II [R = 2-pyridyl, 2,4-(MeO)2C6H3; X = NOH] were obtained in 65 and 60% yield, resp.; II (X = O) with polyphosphoric acid at 130° gave 62-80% indenoisoxazoles III (R = 4-ClC6H4, 4-BrC6H4, 3-pyridyl, Ph, 6-methoxy-2-naphthyl). In preliminary pharmacol. tests with rats, I (R = 3-pyridyl) revealed some analgesic and myorelaxation activity and low toxicity.
IT **16565-60-9P 36288-34-3P 104816-48-0P**
**104816-49-1P 104816-50-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16565-60-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-phenyl- (8CI, 9CI) (CA INDEX NAME)



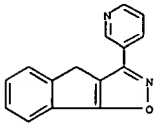
L26 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 36288-34-3 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 104816-48-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(4-bromophenyl)- (9CI) (CA INDEX NAME)

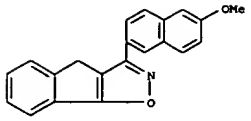


RN 104816-49-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)

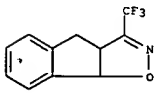


RN 104816-50-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(6-methoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)

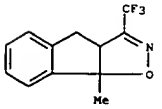
L26 ANSWER 12 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



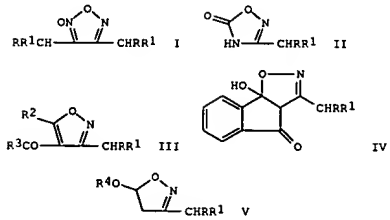
L26 ANSWER 13 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1986:109520 CAPLUS
DOCUMENT NUMBER: 104:109520
TITLE: A competition between 1,3-dipolar cycloaddition and substitution of trifluoroacetonitrile oxide
AUTHOR(S): Tanaka, Kiyoshi; Masuda, Hideyuki; Mitsuhashi, Keiryo
CORPORATE SOURCE: Dep. Ind. Chem., Seikei Univ., Musashino, 180, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1985), 58(7), 2061-5
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:109520
AB Reactions of F3CCNO with conjugated olefins such as styrenes, indenes, and CH2:CRCR1:CHR2 (R = R1 = H, R2 = Me; R = Me, R1 = R2 = H; R = R1 = Me, R2 = H) gave not only the isoxazoline cycloadducts but also linear isomeric oximes. Me or Ph group attached to the unsatd. carbon of the dipolarophiles favored the formation of oxime. Similar competitions were also studied with cyclopentadiene and 1,3-cyclohexadiene where the competitive ratio of the products depended on the ring size.
IT **100695-92-9P 100695-93-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 100695-92-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



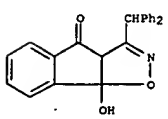
RN 100695-93-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-8b-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L26 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:120973 CAPLUS
DOCUMENT NUMBER: 100:120973
TITLE: 1,3-Dipolar cycloaddition of some diphenylacethydroximic acid chlorides
AUTHOR(S): Kaminski, Jerzy; Eckstein, Zygmunt
CORPORATE SOURCE: Inst. Org. Chem. Technol., Polytech. Univ., Warsaw, 00662, Pol.
SOURCE: Polish Journal of Chemistry (1982), 56(1), 221-8
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:120973
GI

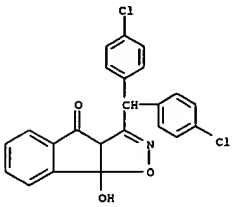


AB Reaction of RR1CHCCl:NOH (R, R1 = Ph, substituted Ph) with acid gave furoxanes I, whereas with KOCN oxadiazoles II were obtained. Isoxazoles III (R2 = R3 = Me, R2R3 = CH2CMe2CH2) were formed from RR1CHCCl:NOH and R2COCH2COR3. Reaction with indandione similarly gave IV. Reaction of RR1CHCCl:NOH with R4OCH:CH2 (R4 = substituted Ph, 2-naphthyl) gave isoxazole V.
IT **89249-60-5P 89249-61-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 89249-60-5 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-(diphenylmethyl)-3a,8b-dihydro-8b-hydroxy- (9CI) (CA INDEX NAME)

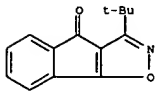


RN 89249-61-6 CAPLUS

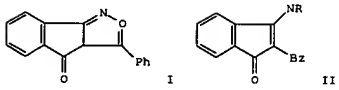
L26 ANSWER 14 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-[bis(4-chlorophenyl)methyl]-2a,8b-dihydro-8b-hydroxy- (9CI) (CA INDEX NAME)



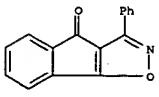
L26 ANSWER 15 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:34042 CAPLUS
DOCUMENT NUMBER: 100:34042
TITLE: Structure elucidation using signal intensity effects in carbon-13 nuclear magnetic resonance
AUTHOR(S): Shapiro, M. J.; Kolpak, M. X.; Lemke, T. L. L.
CORPORATE SOURCE: Dep. Pharm. Med. Chem., Sandoz Inc., East Hanover, NJ, 07936, USA
SOURCE: Journal of Organic Chemistry (1984), 49(1), 187-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Methods for structure elucidation utilizing the perturbation of non-protonated carbon signal intensities are presented. The effects of exchange deuteration and the techniques of difference heteronuclear NOE are described.
IT **82501-33-5**
RL: PRP (Properties)
(structure elucidation of, proton-decoupled carbon-13 NMR and difference heteronuclear NOE in relation to)
RN 82501-33-5 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



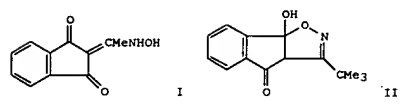
L26 ANSWER 16 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:612439 CAPLUS
DOCUMENT NUMBER: 99:212439
TITLE: Ring opening reactions of indeno[1,2-c]isoxazolones
AUTHOR(S): Lemke, Thomas L.; Sawhney, Kailash N.
CORPORATE SOURCE: Coll. Pharm., Univ. Houston, Houston, TX, 77004, USA
SOURCE: Journal of Heterocyclic Chemistry (1983), 20(4), 899-901
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:212439
GI



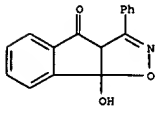
AB Nucleophilic attack of 8-substituted indeno[1,2-c]isoxazol-7-ones and 3-phenylindeno[1,2-c]isoxazol-4-one by Me2SO or PPh3 results in cleavage of the N-O bond of the isoxazole ring leading to the formation of sulfoximides and phosphazenes. Thus, treating indenoisoxazolone I with Me2SO and PPh3 gave II (R = NSOMe2, NPPh3), resp.
IT **87885-97-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring cleavage of)
RN 87885-97-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-phenyl- (9CI) (CA INDEX NAME)



L26 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:594134 CAPLUS
DOCUMENT NUMBER: 99:194134
TITLE: Chemistry of β-triketones. 1. Structure of Schiff base intermediates of 2-acyl-1,3-indandiones
AUTHOR(S): Sawhney, Kailash N.; Lemke, Thomas L.
CORPORATE SOURCE: Coll. Pharm., Univ. Houston, Houston, TX, 77004, USA
SOURCE: Journal of Organic Chemistry (1983), 48(23), 4326-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:194134
GI

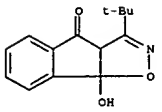


AB Schiff base formation occurs preferentially at the exocyclic carbonyl of 2-acyl-1,3-indandiones. The resulting addition product exists either as an open-chain compound (e.g., I) or a cyclic hemiketal (e.g., II). The size of the acyl substituent influences the structure of the Schiff bases.
IT **62507-92-0P 87206-95-9P 87206-96-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 62507-92-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3a,8b-dihydro-8b-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)

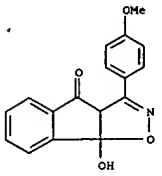


RN 87206-95-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-(1,1-dimethylethyl)-3a,8b-dihydro-8b-hydroxy- (9CI) (CA INDEX NAME)

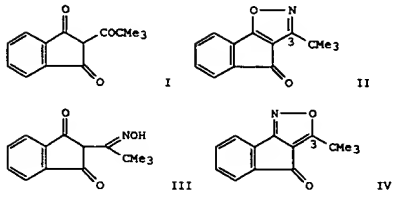
L26 ANSWER 17 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



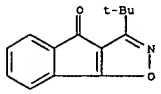
RN 87206-96-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3a,8b-dihydro-8b-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



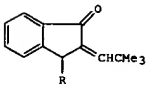
L26 ANSWER 18 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:71358 CAPLUS
DOCUMENT NUMBER: 98:71358
TITLE: The utilization of chemical shift and spin-lattice (T1) relaxation time data for the discrimination of isomeric indenoisoxazoles
AUTHOR(S): Womack, Charles H.; Gampe, Robert T., Jr.; Lemke, B. Kaye; Sawhney, Kailash N.; Lemke, Thomas L.; Martin, Gary E.
CORPORATE SOURCE: Coll. Pharm., Univ. Houston, Houston, TX, 77004, USA
SOURCE: Journal of Heterocyclic Chemistry (1982), 19(5), 1105-7
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



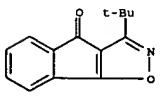
AB Treatment of I with NH2OH under acidic conditions gave II. Similar reaction of I under neutral or basic conditions gave III which was cyclized to IV. 13C NMR was used to differentiate II from IV based on assignments made using T1 relaxation as a guide; in the case of II the C(3) resonance is mediated by both the 14N-13C dipolar mechanism and by the nine Me3C protons while the C(3) of IV is relaxed solely by the Me3C protons. II and IV are also chemical differentiable.
IT **82501-33-5**
RL: PRP (Properties)
(carbon-13 NMR and spin-lattice relaxation of)
RN 82501-33-5 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



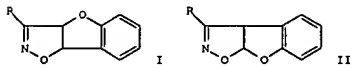
L26 ANSWER 19 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:455721 CAPLUS
DOCUMENT NUMBER: 97:55721
TITLE: Synthesis and chemical reactivity of indenoisoxazoles
AUTHOR(S): Lemke, Thomas L.; Sawhney, Kailash N.; Lemke, B. Kaye
CORPORATE SOURCE: Coll. Pharm., Univ. Houston, Houston, TX, 77004, USA
SOURCE: Journal of Heterocyclic Chemistry (1982), 19(2), 363-8
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:55721
GI



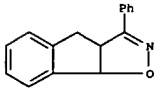
AB Treatment of 2-pivaloyl-1,3-indandione with NH2OH under acidic conditions,
results in formation of 8-tert-butylindeno[1,2-c]isoxazol-7-one (I) while at neutral or basic pH 3-tert-butylindeno[1,2-c]isoxazol-4-one was obtained. The latter compound was readily reduced to amine with N2H4 or H-Pt. The amine, although quite unreactive, was converted to 3-tert-butylindeno[1,2-c]pyrazol-4-one with N2H4 or reduced to II (R = H, OH) with Na-NH3-Me3COH. Surprisingly, the amine obtained from I gave II (R = H) from a Na-NH3 reduction Spectral evidence for each of the structures
is discussed.
IT **82501-33-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 82501-33-5 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



L26 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:475171 CAPLUS
DOCUMENT NUMBER: 89:75171
TITLE: Selectivity in cycloadditions. 6. Cycloadditions of nitrile oxides to benzofuran. Regiochemistry
AUTHOR(S): Caramella, P.; Cellerino, G.; Houk, K. N.; Albini, F. Marinone; Santiago, Cielo
CORPORATE SOURCE: Dep. Chem., Louisiana State Univ., Baton Rouge, LA, USA
SOURCE: Journal of Organic Chemistry (1978), 43(15), 3006-10
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

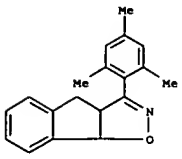


AB Cycloaddn. of RCNO (I; R = Ph, 2,4,6-Me3C6H2) to benzofuran yielded the 2 regioisomeric cycloadducts in 70:30 and 26:74 ratio, resp. Frontier-orbital considerations, using ab initio STO-3G, CNDO/2 or EHMO calcns., and a comparison with the regioselectivities observed with indene
and styrene allowed elucidation of the inversion of regiochem. of the cycloaddns. of I to benzofuran.
IT **27271-35-8P 61191-73-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27271-35-8 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



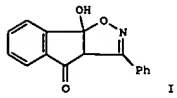
RN 61191-73-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 20 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L26 ANSWER 21 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:155036 CAPLUS
DOCUMENT NUMBER: 86:155036
TITLE: Structure and properties of 2-acyl-1,3-indandione oximes
AUTHOR(S): Geita, L.; Dalberga, I.; Grinvalde, A.
CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija
(1976), (6), 704-7
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 86:155036
GI

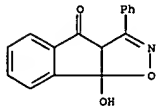


I

AB IR studies showed that the monooximes of 2-acetyl-1,3-indandione, its 4-NO2, 4-NH2, 4-OH, and 4-AcNH derivs., and 2-propionyl-1,3-indandione existed in the enol form and were strongly associated; that of 2-benzoyl-1,3-indandione had the cyclic structure I.

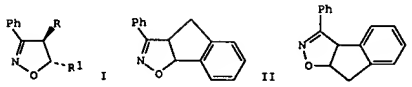
IT **62507-92-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

RN 62507-92-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3a,8b-dihydro-8b-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)



L26 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:4459 CAPLUS
DOCUMENT NUMBER: 86:4459
TITLE: Δ2-Isoxazoline derivatives. Part X. 1,3-Dipolar cycloadditions of nitrones and nitrile oxides with indene, 1,2-dihydrodnaphthalene, and trans-1-phenylpropene
AUTHOR(S): Bianchi, Giorgio; De Micheli, Carlo; Gandolfi, Remo
CORPORATE SOURCE: Ist. Chim. Org., Univ. Pavia, Pavia, Italy
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (14), 1518-23
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

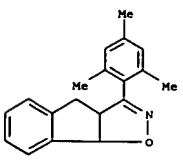


I II III

AB Reaction of cyclic and acyclic nitrones and nitrile oxides with 1,2-dihydronaphthalene, indene, and trans-MeCH:CHPh gave mixts. of regioisomers. E.g., PhC.tplbond.NO with trans-MeCH:CHPh gave 43.5% of a 66:34 mixture of isoxazolines I (R = Me, R1 = Ph; R = Ph, R1 = Me) and with indene 91% of a 98:2 mixture of II and III was formed. The results are analyzed on the basis of frontier orbital interactions and steric requirements of the reagents; transition state structures for the reactions are proposed.

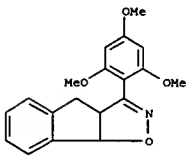
IT **61191-73-9P 61191-75-1P 61246-84-2P 61246-85-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 61191-73-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



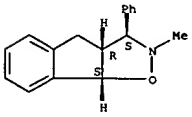
RN 61191-75-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(2,4,6-trimethoxyphenyl)- (9CI)

L26 ANSWER 22 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(CA INDEX NAME)



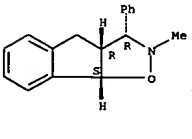
RN 61246-84-2 CAPLUS
CN 2H-Indeno[2,1-d]isoxazole, 3,3a,4,8b-tetrahydro-2-methyl-3-phenyl-, (3α,3aα,8bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



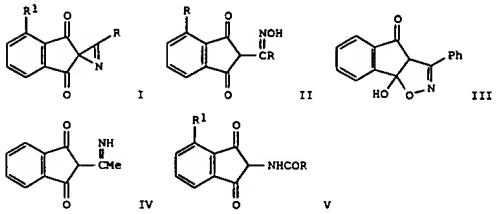
RN 61246-85-3 CAPLUS
CN 2H-Indeno[2,1-d]isoxazole, 3,3a,4,8b-tetrahydro-2-methyl-3-phenyl-, (3α,3aβ,8bβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L26 ANSWER 23 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:420963 CAPLUS
DOCUMENT NUMBER: 85:20963
TITLE: Synthesis and study of 2,3'-spiro[(indan-1,3-dione)-1'-azirines] and products of their opening
AUTHOR(S): Geita, L.; Dalberga, I.; Grinvalde, A.; Jankovska, I.
CORPORATE SOURCE: Inst. Org. Sint., Riga, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1976), (1), 65-9
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 85:20963
GI

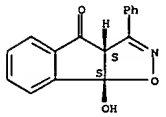



AB The title spiro compds. I (R = Me, Et, Pr; R1 = H, NO2) were prepared by cyclization of the acylindandione oximes II in HOAc-Ac2O or in acetone containing 4-MeC6H4SO2Cl; I (R = Ph; R1 = H) was prepared by rearrangement of III. Reduction of I (R = Me; R1 = H) by HI gave the imine IV, whereas ring cleavage of I in aqueous NaOH gave the indanyl amides V.

IT **59525-95-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, spiro[indan-azirine] from)

RN 59525-95-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazol-4-one, 3a,8b-dihydro-8b-hydroxy-3-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L26 ANSWER 23 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

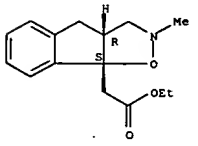
L26 ANSWER 24 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:569425 CAPLUS
DOCUMENT NUMBER: 81:169425
TITLE: Tricyclic analogs of the prodines
AUTHOR(S): Menard, Marcel; Rivest, Pierre; Morris, Lee; Meunier, Jacques; Perron, Yvon G.
CORPORATE SOURCE: Bristol Lab. Canada, Candiac, QC, Can.
SOURCE: Canadian Journal of Chemistry (1974), 52(12), 2316-26
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Benzisoquinolines I (R = H, COEt; R1 = R2 = H; R1 = Me, R2 = H, 7-OMe, 9-OMe; R3 = H, Me) were prepared as prodine and benzomorphan analogs. I (R = H) were obtained by cycloaddn. of Et 3,4-dihydro-1-naphthylacetate with CH2:N(:O)Me, reductive cleavage of the isoxazolidine ring, cyclization of the amino esters, and reduction of the lactam O. I (R = Me) were prepared by treating tetralones II (R4R5 = O) with LiCH2CN, reducing II (R4 = OH, R5 = CH2CN)to I (R = R3 = H, R1 = Me, R2 = H, 7-OMe, 9-OMe), which were methylated and esterified. I (R = COEt, R1 = R2 = H, R3 = Me; R = H, R1 = Me, R2 = 7-OMe, R3 = H, Me; R = COEt, R1 = R3 = Me, R2 = H, 7-OMe, 9-OMe) had analgesic ED50 3-32 mg/kg s.c. in mice. Methylation of I (R = R, R1 = Me, R2 = 7-OMe, R3 = H) decreased the analgesic ED50 from 30 to 3 mg/kg. I (R = H, COEt, R1 = R2 = H, R3 = Me) had antidepressant ED50 in the reserpine hypothermic test in mice of 1 mg/kg orally.

IT **54125-42-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive cleavage of)

RN 54125-42-7 CAPLUS
CN 8bH-Indeno[2,1-d]isoxazole-8b-acetic acid, 2,3,3a,4-tetrahydro-2-methyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

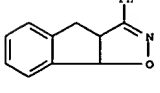


L26 ANSWER 25 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:465646 CAPLUS
DOCUMENT NUMBER: 79:65646
TITLE: Selectivity in cycloadditions. III. Regioselectivity and π-conjugation in the 1,3-dipolar cycloadditions of benzonitrile oxide
AUTHOR(S): Bailo, Giorgio; Caramella, Pierluigi; Cellerino, Giuseppe; Invernizzi, Anna G.; Gruenanger, Paolo
CORPORATE SOURCE: Ist. Chim. Org., Univ. Pavia, Pavia, Italy
SOURCE: Gazzetta Chimica Italiana (1973), 103(1-2), 47-59
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Treatment of benzohydroxamic acid chloride with Et3N in Et2O at 0° gave PhC.tplbond.NO which cyclo-added to cyclopentadiene to give 94% of a mixture of monoadducts containing 99% I and 1% II. Further cycloaddn. of PhC.tplbond.NO to I give a mixture containing 30% anti-III, 45% anti-IV, 6% syn-III, and 19% syn-IV. Similarly, cycloaddn. to II give a mixture containing 39% anti-IV, 43% anti-V, 18% syn-IV, and 0% syn-V. The cycloaddn. of PhC.tplbond.NO to indene also gave a mixture containing 98% VI and 2% VII. The π-configurative control of the highly regioselective cycloaddn. of PhC.tplbond.NO to cyclopentadiene and indene was contrasted to the lack of regiospecificity or -selectivity in the cycloaddn. of PhC.tplbond.NO to 6,6-dimethyl- and 6,6-diphenylfulvene. The frontier orbital interactions of PhC.tplbond.NO with indene and cyclopentadiene were discussed.

IT **27271-35-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

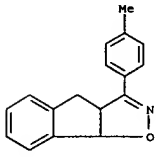
RN 27271-35-8 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



L26 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:405352 CAPLUS
DOCUMENT NUMBER: 79:5352
TITLE: 1,2-Disubstituted indene compounds
INVENTOR(S): Trepanier, Donald L.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: U.S., 6 pp. Division of U.S. 3,636,116 (CA;112961q).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

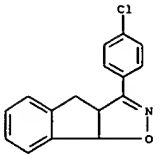
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 3719674 | A | 19730306 | US 1971-113744 | 19710208 |
| US 3636116 | A | 19720118 | US 1968-757102 | 19680903 |
| PRIORITY APPLN. INFO.: | | | US 1968-757102 | A3 19680903 |

GI For diagram(s), see printed CA Issue.
AB The indeno[2,1-d]isoxazoles (I, R = Cl, R1 = H; R = Me, R1 = H; R = R1 = H, Cl were prepared by treating benzylhydroxamic acid chlorides with indene.
LiAlH4 reduction of I gave the aminobenzylindanols II. II (R = Cl, R1 = H)
was treated with NaOAc and BrCN to give [4-chloro-α-(1-hydroxy-2-indanyl)benzylcyanamide, which was treated with HCl to give the indeno[2,1-e][1,3]oxazine (III, R = Cl). III (R = H, Me) were similarly prepared. Mice rejected with I (R = R1 = H) (500 mg/kg and 100 mg/kg of hexabarbital slept more than twice as long as those treated only with hexabarbital. At 34 mg/kg II (R = Cl) protected mice from electroshock seizures. III (R = H) potentiated the hyperexcitement effects of d-amphetamine in mice.
IT **26718-19-4P 26718-32-1P 27271-35-8P 27271-38-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26718-19-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

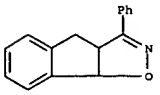



RN 26718-32-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(4-chlorophenyl)-3a,8b-dihydro- (9CI) (CA INDEX NAME)

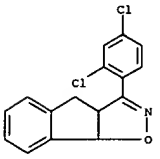
L26 ANSWER 26 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)




RN 27271-35-8 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



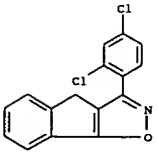

RN 27271-38-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(2,4-dichlorophenyl)-3a,8b-dihydro- (8CI, 9CI) (CA INDEX NAME)




L26 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:112961 CAPLUS
DOCUMENT NUMBER: 76:112961
TITLE: Pharmacologically active 1,2-substituted indene compounds
INVENTOR(S): Trepanier, Donald L.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

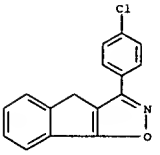
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 3636116 | A | 19720118 | US 1968-757102 | 19680903 |
| US 3719674 | A | 19730306 | US 1971-113744 | 19710208 |
| PRIORITY APPLN. INFO.: | | | US 1968-757102 | A3 19680903 |

GI For diagram(s), see printed CA Issue.
AB Treatment of indene with substituted chlorobenzohydroxamoyl chlorides gave
indenoisoxazoles (I, R1, R2, R3 = H, Cl, Br, Me), which were reduced to 2-(α-aminosubstituted benzyl)-1-indanols, which when treated with BrCN and cyclized, gave the indenooxazines (II, R1, R2, R3 = H, Cl, Br, Me). The compds. were amphetamine and barbiturate potentiators. Thus, Et3N was added to CHCl3 containing 4-chloro-benzohydroxamoyl chloride and indene and the mixture refluxed to give I (R1 = R3 = H, R2 = 4-Cl) (III). III was reduced by LiAlH4 in Et2O to give 2-(α-amino-4-chlorobenzyl)-1-indanol, which when administered to mice at 65 mg/kg with hexobarbital, doubled the mice sleep time. Five other I, 3 indanols, 3 BrCN-indanol reaction products, and 4 II were prepared
IT **36288-38-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36288-38-7 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(2,4-dichlorophenyl)- (9CI) (CA INDEX NAME)




IT **36288-34-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
RN 36288-34-3 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

L26 ANSWER 27 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

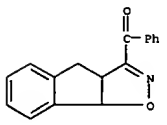


L26 ANSWER 28 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1971:141643 CAPLUS
DOCUMENT NUMBER: 74:141643
TITLE: Heteroaromaticity. XLIV. Reactivities of benzoyl cyanide N-oxide and some derivatives therefrom
AUTHOR(S): Sasaki, Tadashi; Yoshioka, Toshiyuki; Suzuki, Yasuyuki
CORPORATE SOURCE: Inst. Appl. Org. Chem., Nagoya Univ., Nagoya, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1971), 44(1), 185-9
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 74:141643

AB o-Chloroisonitrosoacetophenone (I) was treated with ethylenic and acetylenic dipolarophiles to give 3-benzoylisoxazolidines and -isoxazoles, resp. With m-nitrobenzonitrile, I yielded 3-benzoyl-5-(m-nitrophenyl)-1,2,4-oxadiazole. The phenylhydrazones of the 3-benzoylisoxazole and -oxodiazole thus produced were converted into the corresponding 1,2,3-triazoles thermally or by treatment with a base. The photoinduced rearrangement of 3-benzoyl-5-phenylisoxazole gave 2-benzoly-5-phenyloxazole. Treatment of I with aziridine gave an aziridine oxime, which was converted into 2-benzoyloxazoline.

IT **31879-30-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 31879-30-8 CAPLUS
CN Ketone, 3a,8b-dihydro-4H-indeno[2,1-d]isoxazol-3-yl phenyl (8CI) (CA INDEX NAME)

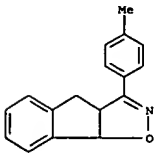


L26 ANSWER 29 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1970:435300 CAPLUS
DOCUMENT NUMBER: 73:35300
TITLE: Synthesis and screening for antideperessant activity of some aminoindanooxazolines, aminoindanooxazines, and aminoacenaphthoxazolines
AUTHOR(S): Trepanier, Donald L.; Faith, H. Eldridge; Eble, John N.
CORPORATE SOURCE: Chem. Res. and Pharmacol. Dep., Dow Chem. Co., Zionsville, IN, USA
SOURCE: Journal of Medicinal Chemistry (1970), 13(4), 729-33
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

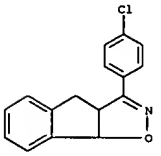
AB Some aminoindanooxazolines, aminoindanooxazines, and aminoacenaphthoxazolines with spatial orientations similar to those of the tricyclic drugs were synthesized and tested for potential antidepressant activity. None were able to prevent reserpine ptosis. Some potentiated d-amphetamine toxicity and prolonged hexobarbital sleep time in mice.

IT **26718-19-4 26718-32-1 27271-35-8 27271-38-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(antidepressants)

RN 26718-19-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

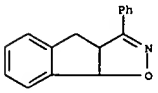


RN 26718-32-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(4-chlorophenyl)-3a,8b-dihydro- (9CI) (CA INDEX NAME)

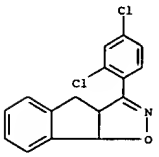


RN 27271-35-8 CAPLUS

L26 ANSWER 29 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 27271-38-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(2,4-dichlorophenyl)-3a,8b-dihydro- (8CI, 9CI) (CA INDEX NAME)



L26 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1970:43542 CAPLUS
DOCUMENT NUMBER: 72:43542
TITLE: Heteroaromaticity. XXXV. Thermal 1,3-cycloaddition of aromatic hydroxamoyl chlorides with cyclic olefins
AUTHOR(S): Sasaji, Tadashi; Yoshioka, Toshiyuki; Suzuki, Yasuyuki
CORPORATE SOURCE: Nagoya Univ., Nagoya, Japan
SOURCE: Yuki Gosei Kagaku Kyokaishi (1969), 27(10), 998-9
CODEN: YGKKAE; ISSN: 0037-9980
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

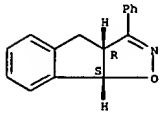
GI For diagram(s), see printed CA Issue.

AB 5-Nitro-2-furanhydroxamoyl chloride (I) (0.95 g) and 0.75 g acenaphthylene in 30 ml PhMe were refluxed 10 hr to give 0.3 g II (R1 = 5-nitro-2-furyl), m. 208-9° (C6H6). Similarly, the following II were prepared (R1, m.p., and % yield given): p-O2NC6H4, 274-6°, 50; m-O2N-C6H4, 164-6°, 50; and Ph, 207-9°, 6 0. Similar treatment of I with indene gave 80% III (R2 = 5-nitro-2-furyl ), m. 234-6°. Similarly, the following III were prepared (R2, m.p., and % yield given):
p-O2NC6H4, 222-4°, 65; m-O2NC6H4, 148-50°, 65; and Ph, 139-41°, 45. They were shown to have a common isoxazoline structure on the basis of the anal. and spectral data.

IT **20087-23-4P 25471-27-6P 25471-28-7P 25471-29-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 20087-23-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl-, cis- (8CI) (CA INDEX NAME)

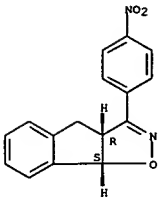
Relative stereochemistry.



RN 25471-27-6 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(p-nitrophenyl)- (8CI) (CA INDEX NAME)

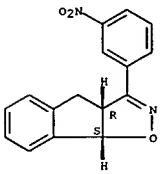
Relative stereochemistry.

L26 ANSWER 30 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



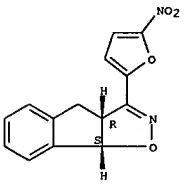
RN 25471-28-7 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(m-nitrophenyl)- (8CI) (CA INDEX NAME)

Relative stereochemistry.

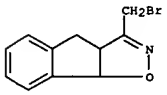


RN 25471-29-8 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-(5-nitro-2-furyl)- (8CI) (CA INDEX NAME)

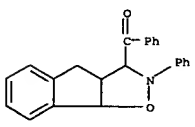
Relative stereochemistry.



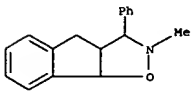
L26 ANSWER 31 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:476043 CAPLUS
DOCUMENT NUMBER: 71:76043
TITLE: Molecular spectroscopy
AUTHOR(S): Rollier, Mario A.
CORPORATE SOURCE: Univ. Pavia, Pavia, Italy
SOURCE: Corsi e Seminari di Chimica, Consiglio Nazionale delle Ricerche e Fondazione F. Giordani (1968), No. 14, 92-3
CODEN: CSECB7; ISSN: 0579-0670
DOCUMENT TYPE: Journal
LANGUAGE: Italian
AB An account is given of work relating to the spectral anal. of 2-isoxazole derivs. and to N.M.R. applications for determination of partition coeffs. of BF3 between various solvents and for H-bond investigation.
IT **24383-88-8**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, spectrochem.)
RN 24383-88-8 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-(bromomethyl)-3a,8b-dihydro- (8CI) (CA INDEX NAME)



L26 ANSWER 32 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:115043 CAPLUS
DOCUMENT NUMBER: 70:115043
TITLE: 1,3-Dipolar cycloaddition. L. Characterization of unsaturated compounds as acylnitrone adducts
AUTHOR(S): Huisgen, Rolf; Hauck, Hans; Seidl, Helmut; Burger, Monika
CORPORATE SOURCE: Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1969), 102(4), 1117-28
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 70:115043
GI For diagram(s), see printed CA Issue.
AB p-RC6H4COCH:N+PhO- (I) (R = H or NO2) reacted rapidly with unsatd. compds., such as α,β-unsatd. carboxylic acid esters, ketones, and nitriles to give crystalline 1,3-cycloadducts. Thus, the reaction of I (R = H) with CH2:CHCO2Me gave Me 2-phenyl-3-benzoylisoxazolidine-5-carboxylate (II). 2-Phenylisatogen was less suited for the characterization of C-C double bonds.
IT **22269-80-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22269-80-3 CAPLUS
CN Ketone, phenyl 3,3a,4,8b-tetrahydro-2-phenyl-2H-indeno[2,1-d]isoxazol-3-yl- (8CI) (CA INDEX NAME)

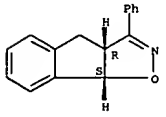


L26 ANSWER 33 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:452052 CAPLUS
DOCUMENT NUMBER: 69:52052
TITLE: 1,3-Dipolar cycloadditions. XLII. Nitrone additions to other aryl-conjugated ethylenes and vinyl ethers
AUTHOR(S): Huisgen, Rolf; Grashey, Rudolf; Seidl, Helmut; Hauck, Hans
CORPORATE SOURCE: Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1968), 101(7), 2559-67
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 69:52052
AB α-Methylstyrene and 1,1-diphenylethylene added to nitrones to give 5,5-disubstituted-isoxazolidines. Their structures were established by N.M.R. and chemical degradation methods. Similar adducts were obtained with 2-vinyl-pyridine, indene, 1,2-dihydronaphthalene, acenaphthylene, and with alkoxy-substituted ethylenes, such as butyl vinyl ether.
IT **19380-34-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19380-34-8 CAPLUS
CN 2H-Indeno[2,1-d]isoxazole, 3,3a,4,8b-tetrahydro-2-methyl-3-phenyl- (8CI) (CA INDEX NAME)

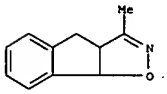


L26 ANSWER 34 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:427307 CAPLUS
DOCUMENT NUMBER: 69:27307
TITLE: NMR spectra of 2-isoxazolines. II. Cis-trans isomers of 4,5-disubstituted 2-isoxazolines
AUTHOR(S): Aversa, Maria Chiara; Cum, Giampietro; Crisafulli, Maria
CORPORATE SOURCE: Univ. Messina, Messian, Italy
SOURCE: Gazzetta Chimica Italiana (1968), 98(1), 42-7
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB N.M.R. data for compds. of the general formula cis-I and trans-I and compound II in CDCl3 are obtained and are useful for structure assignment.
trans-3,4,5-Triphenyl-2-isoxazoline, and the following trans-I (R and R1 given) are prepared: CO2Me, Ph; CO2Et, Ph; CO2Me, CO2Me; CO2CH2Ph, CO2CH2Ph;
tert-BuCO, Ph; Ac, Ph,; Ac, p-O2N6H4; p-O2NC6H4, Ac; Bz, o-O2NC6H4; Bz, p-O2NC6H4; p-O2NC6H4, Bz. Also prepared were II and the following cis-I (R
and R1 given) according to known methods: Ph, Ph; Ph, CO2Me; CO2Et, Ph; CO2Me; CO2CH2Ph, CO2CH2Ph.
IT **20087-23-4**
RL: PRP (Properties)
(nuclear magnetic resonance of)
RN 20087-23-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl-, cis- (8CI) (CA INDEX NAME)

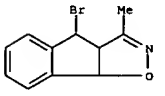
Relative stereochemistry.



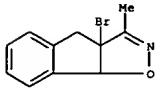

L26 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:500043 CAPLUS
DOCUMENT NUMBER: 67:100043
TITLE: Indenoisoxazole derivatives
AUTHOR(S): Bianchi, Giorgio; Gandolfi, Remo; Gruenanger, Paolo; Perotti, Angelo
CORPORATE SOURCE: Univ. Pavia, Pavia, Italy
SOURCE: Journal of the Chemical Society [Section] C: Organic (1967), (17), 1598-602
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:100043
GI For diagram(s), see printed CA Issue.
AB From the cycloaddn. of acetonitrile N-oxide with indene two isomeric methyldihydroindenoisoxazoles (I and II) were isolated. Elucidation of their structures by bromination and 1H N.M.R. spectroscopy, and related reactions on analogous compds. are described. 17 references.
IT **16565-52-9P 16565-54-1P 16565-55-2P**
**16565-56-3P 16565-57-4P 16565-58-5P**
**16565-60-9P 16565-61-0P 16565-62-1P**
**16565-71-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16565-52-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-methyl- (8CI) (CA INDEX NAME)




RN 16565-54-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 4-bromo-3a,8b-dihydro-3-methyl- (8CI) (CA INDEX NAME)

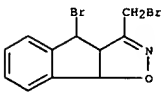



RN 16565-55-2 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a-bromo-3a,8b-dihydro-3-methyl- (8CI) (CA INDEX NAME)

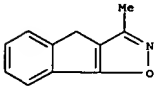



L26 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 16565-56-3 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 4-bromo-3-(bromomethyl)-3a,8b-dihydro- (8CI) (CA INDEX NAME)



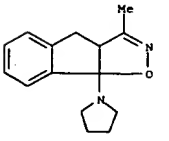

RN 16565-57-4 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-methyl- (8CI) (CA INDEX NAME)




RN 16565-58-5 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-methyl-8b-(1-pyrrolidinyl)-, monomethiodide (8CI) (CA INDEX NAME)

CM 1

CRN 46849-31-4
CMF C15 H18 N2 O



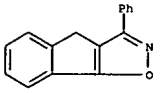

CM 2

CRN 74-88-4
CMF C H3 I

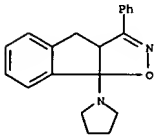
H3C—I

RN 16565-60-9 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3-phenyl- (8CI, 9CI) (CA INDEX NAME)

L26 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



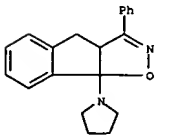

RN 16565-61-0 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl-8b-(1-pyrrolidinyl)- (8CI) (CA INDEX NAME)




RN 16565-62-1 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl-8b-(1-pyrrolidinyl)-, monomethiodide (8CI) (CA INDEX NAME)

CM 1

CRN 16565-61-0
CMF C20 H20 N2 O



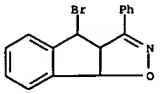

CM 2

CRN 74-88-4
CMF C H3 I

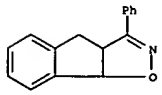
H3C—I

RN 16565-71-2 CAPLUS

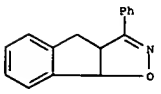
L26 ANSWER 35 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 4H-Indeno[2,1-d]isoxazole, 4-bromo-3a,8b-dihydro-3-phenyl- (8CI) (CA INDEX NAME)




L26 ANSWER 36 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1958:6351 CAPLUS
DOCUMENT NUMBER: 52:6351
ORIGINAL REFERENCE NO.: 52:1145b-c
TITLE: Structure of the adduct of benzonitrile oxide to indene, and the synthesis of 1- and 2-benzoylindan
AUTHOR(S): Perold, G. W.; v. Reiche, F. V. K.
CORPORATE SOURCE: S. A. Iron and Steel Ind. Corp., Ltd., Pretoria
SOURCE: Journal of the South African Chemical Institute (1957), 10, 5-10
CODEN: JSACAT; ISSN: 0038-2078
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Refluxing constant-boiling HI cleaves the 2-isoxazoline, obtained by addition of benzonitrile oxide to indene, to 2-benzoylindan. The addition follows the Markownikoff rule and leads to 3-phenyl-4,5-(2,1-indano)-2-isoxazoline. The nature of the cleavage reaction by-products is discussed. A description is made of the synthesis of the 1- and 2-benzoylindans by the reaction of Ph2Cd with the corresponding acid chlorides. 15 references.
IT 27271-35-8, 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (preparation of)
RN 27271-35-8 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



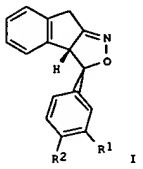

L26 ANSWER 37 OF 37 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1957:34809 CAPLUS
DOCUMENT NUMBER: 51:34809
ORIGINAL REFERENCE NO.: 51:6603f-i
TITLE: Structure of isoxazoline compounds: a spectral study
AUTHOR(S): Perold, G. W.; Steyn, A. P.; v. Reiche, F. V. K.
CORPORATE SOURCE: S. African Iron and Steel Ind. Corp., Ltd., Pretoria
SOURCE: Journal of the American Chemical Society (1957), 79, 462-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 51:34809
AB Cl passed through 10.0 cc. PhCH:NOH in 60 cc. about 8.3N HCl at 0° during 15-20 min. and filtered yielded up to 76% benzhydroximic chloride (I), m. 42-8°. I (10.7 g.) and 7.2 g. styrene in 50 cc. Et2O treated at 0° gradually with 45 cc. 14% aqueous NaOH, and the Et2O solution washed with H2O after 15 min., kept overnight, and evaporated yielded 3,5-diphenyl-2-isoxazoline (II), needles, m. 76° (from EtOH). Similarly were prepared: 5-(p-tolyl) analog of II, m. 94°, 96% yield; 5-Me derivative of II, m. 76°, 60% yield; 3-phenyl-4,5-indano-2-isoxazoline, m. 134° 66% yield; 3-phenyl-4,5-(dicyclopentadieno)-2-oxazoline, m. 110-11°, 40% yield. Ph(CH2)2Bz reduced with LiAlH4 gave 86% Ph(CH2)2CH(OH)Ph (III). III (5.23 g.) and 5.23 g. (CO2H)2 heated 0.5 hr. at 130-80°, kept 2 hrs. at 180°, and chromatographed on Al2O3 yielded 5.0 g. crude product which distilled gave 4.0 g. PhCH:CHCH2Ph, b0.06 120-30° (bath), nD20 1.6000. BzH (20 g.) mixed carefully with 25 g. 33% aqueous MeNH2, the H2O removed azeotropically with C6H6, the liquid residue treated 1.5 hrs. at room temperature with a large excess of NH2OH.HCl and aqueous NaOH, and the product isolated with C6H6 yielded 61% benzylidene methylimine, b42 99-103° (bath), nD17 1.5522. By the method of Janny [Ber. 16, 174 (1833)] were prepared the following compds. PhRC:NOR' [R, R', % yield, and b.p. (bath)/mm. given]: Me, Me, 33, 132-5°/46; Me, PhCH2, 72, 115-19°/0.1; PhCH2CH2, Me, 20, 110°/0.1. The ultraviolet absorption maximum and the infrared absorption maximum in the 1560-1610 cm.-1 region are tabulated.
IT 27271-35-8, 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (preparation of)
RN 27271-35-8 CAPLUS
CN 4H-Indeno[2,1-d]isoxazole, 3a,8b-dihydro-3-phenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



```
=> s l9
L28           2 L9

=> d ibib abs hitstr 1-2
```

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:131886 CAPLUS
DOCUMENT NUMBER: 137:6110
TITLE: Transformation of phthalaldehyde to indenoisoxazole derivatives
AUTHOR(S): Dhar, Mita; Bhattacharjya, Anup
CORPORATE SOURCE: Indian Institute of Chemical Biology, Calcutta, 700032, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2001), 40B(11), 1140-1143
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:6110
GI



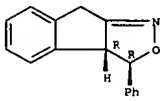
I

AB Phthalaldehyde was converted to 1-stilbenyl-2-nitroethane derivs., which afford 3-arylindenoisoxazoles via silylnitronate or nitrile oxide cycloaddn. reactions. The compds. thus prepared included indenoisoxazoles I (R1 = R2 = H; R1 = OMe, R2 = OCH2Ph).

IT **433214-89-2P 433214-91-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(transformation of phthalaldehyde into 3a,8-dihydro-3-phenyl-3H-indeno[2,1-c]isoxazole derivs.)

RN 433214-89-2 CAPLUS
CN 3H-Indeno[2,1-c]isoxazole, 3a,8-dihydro-3-phenyl-, (3R,3aR)-rel- (9CI) (CA INDEX NAME)

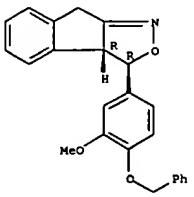
Relative stereochemistry.



RN 433214-91-6 CAPLUS
CN 3H-Indeno[2,1-c]isoxazole, 3a,8-dihydro-3-[3-methoxy-4-(phenylmethoxy)phenyl]-, (3R,3aR)-rel- (9CI) (CA INDEX NAME)

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

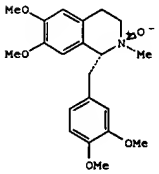
Relative stereochemistry.



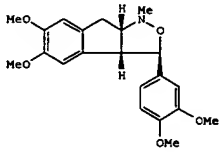
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

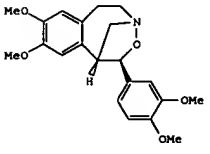
ACCESSION NUMBER: 1980:532663 CAPLUS
DOCUMENT NUMBER: 93:132663
TITLE: The characterization and thermolysis of cis- and trans-(±)-laudanosine N-oxide
AUTHOR(S): Bremner, John B.; Le Van Thuc
CORPORATE SOURCE: Dep. Chem., Univ. Tasmania, Hobart, 7001, Australia
SOURCE: Australian Journal of Chemistry (1980), 33(2), 379-94
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



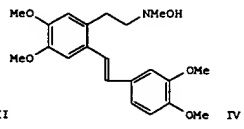
I



II



III



IV

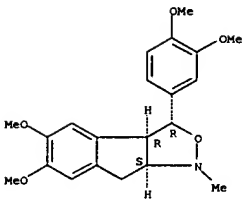
AB The isolation and characterization of cis-(I) and trans-(±)-laudanosine N-oxide is described. Thermolysis of I afforded the new fused and bridged heterocyclic derivs. II and III. Other products included (±)-laudanosine, the Cope elimination product, IV, and 1-(3,4-dimethoxybenzyl)-7,8-dimethoxy-3-methyl-1,3,4,5-tetrahydro-2,3-benzoxazepine, the product of a Meisenheimer rearrangement. By contrast, trans-(±)-laudanosine N-oxide gave IV in nearly quant. yield. Some of the possible mechanistic implications of these results are discussed.

IT **74904-75-9P 74904-76-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 74904-75-9 CAPLUS
CN 1H-Indeno[2,1-c]isoxazole, 3-(3,4-dimethoxyphenyl)-3,3a,8,8a-tetrahydro-5,6-dimethoxy-1-methyl-, (3α,3aα,8aα)- (9CI) (CA INDEX NAME)

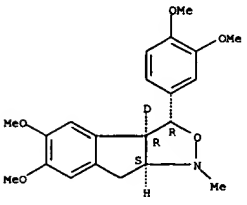
Relative stereochemistry.

L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 74904-76-0 CAPLUS
CN 1H-Indeno[2,1-c]isoxazole, 3-(3,4-dimethoxyphenyl)-3,3a,8,8a-tetrahydro-3a-d-5,6-dimethoxy-1-methyl-, (3α,3aα,8aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



```
=> s l15
L29           7 L15

=> d ibib abs hitstr 1-7
```

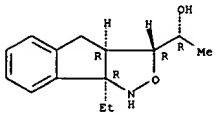
L29 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:252046 CAPLUS
DOCUMENT NUMBER: 142:482283
TITLE: Succinct Synthesis of β-Amino Acids via Chiral Isoxazolines
AUTHOR(S): Fuller, Amelia A.; Chen, Bin; Minter, Aaron R.; Mapp, Anna K.
CORPORATE SOURCE: Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109-1055, USA
SOURCE: Journal of the American Chemical Society (2005), 127(15), 5376-5383
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB β-Amino acids are important synthetic targets due to their presence in a wide variety of natural products, pharmaceutical agents, and mimics of protein structural motifs. While β-amino acids containing geminal substitution patterns have enormous potential for application in these contexts, synthetic challenges to the stereoselective preparation of this class of compound have thus far limited more complete studies. A straightforward method is presented, employing chiral isoxazolines as key intermediates to access five different β-amino acid structural types with excellent selectivity. Of particular note is the use of this approach to prepare highly substituted cis-β-proline analogs. The ready access to these diversely substituted compds. is expected to facilitate future studies of the structure and function of this important class of mols.

IT **851985-42-7P 851985-46-1P 851985-50-7P**
**851985-62-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(succinct synthesis of β-amino acids via chiral isoxazolines)

RN 851985-42-7 CAPLUS
CN 1H-Indeno[1,2-c]isoxazole-3-methanol, 8b-ethyl-3,3a,4,8b-tetrahydro-α-methyl-, (αR,3R,3aR,8bR)-rel- (9CI) (CA INDEX NAME)

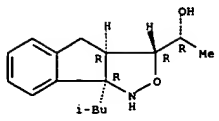
Relative stereochemistry.



RN 851985-46-1 CAPLUS
CN 1H-Indeno[1,2-c]isoxazole-3-methanol, 3,3a,4,8b-tetrahydro-α-methyl-8b-(2-methylpropyl)-, (αR,3R,3aR,8bR)-rel- (9CI) (CA INDEX NAME)

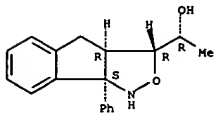
Relative stereochemistry.

L29 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



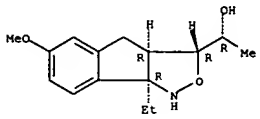
RN 851985-50-7 CAPLUS
CN 1H-Indeno[1,2-c]isoxazole-3-methanol, 3,3a,4,8b-tetrahydro-α-methyl-8b-phenyl-, (αR,3R,3aR,8bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 851985-62-1 CAPLUS
CN 1H-Indeno[1,2-c]isoxazole-3-methanol, 8b-ethyl-3,3a,4,8b-tetrahydro-6-methoxy-α-methyl-, (αR,3R,3aR,8bR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

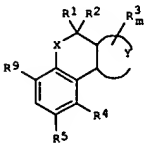


REFERENCE COUNT: 100 THERE ARE 100 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

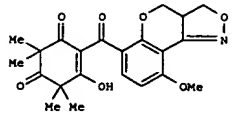
L29 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:861685 CAPLUS
DOCUMENT NUMBER: 134:29409
TITLE: Preparation of tricyclic aroylcyclohexanediones as herbicides
INVENTOR(S): Witschel, Matthias; Kudis, Steffen; Langemann, Klaus; Baumann, Ernst; Von Deyn, Wolfgang; Mayer, Guido; Misslitz, Ulf; Neidlein, Ulf; Otten, Martina; Westphalen, Karl-Otto; Walter, Helmut
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000073311 | A2 | 20001207 | WO 2000-EP4806 | 20000526 |
| WO 2000073311 | A3 | 20010419 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2372241 | AA | 20001207 | CA 2000-2372241 | 20000526 |
| EP 1181295 | A2 | 20020227 | EP 2000-940273 | 20000526 |
| EP 1181295 | B1 | 20040218 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| BR 2000011109 | A | 20020319 | BR 2000-11109 | 20000526 |
| JP 2003501359 | T2 | 20030114 | JP 2001-500636 | 20000526 |
| AT 259816 | E | 20040315 | AT 2000-940273 | 20000526 |
| AU 782843 | B2 | 20050901 | AU 2000-55260 | 20000526 |
| US 6583089 | B1 | 20030624 | US 2001-979991 | 20011129 |
| ZA 2001009886 | A | 20021202 | ZA 2001-9886 | 20011130 |
| PRIORITY APPLN. INFO.: | | | DE 1999-19925103 A | 19990601 |
| | | | WO 2000-EP4806 W | 20000526 |

OTHER SOURCE(S): MARPAT 134:29409
GI



I



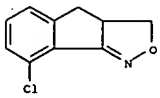
II

L29 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

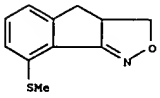
AB Title compds. [I; RR3 = atoms to complete an (un)substituted heterocyclic or -heteroarom. ring; R1,R2 = H, halo, alkyl; alkoxy, etc.; R5 = H, halo, alkyl; R9 = e.g., (un)substituted 2-hydroxy-6-oxocyclohexen-1-ylcarbonyl; Z = bond, O, SO0-2, CH2, (alkyl)imino, etc.] were prepared as herbicides (no data). Thus, Me 2-hydroxy-4-methoxybenzoate was converted in 7 steps to title compound II.

IT **293312-27-3P 293312-28-4P 293312-29-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tricyclic aroylcyclohexanediones as herbicides)

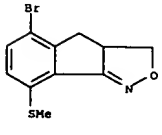
RN 293312-27-3 CAPLUS
CN 3H-Indeno[1,2-c]isoxazole, 8-chloro-3a,4-dihydro- (9CI) (CA INDEX NAME)



RN 293312-28-4 CAPLUS
CN 3H-Indeno[1,2-c]isoxazole, 3a,4-dihydro-8-(methylthio)- (9CI) (CA INDEX NAME)



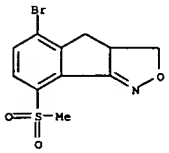
RN 293312-29-5 CAPLUS
CN 3H-Indeno[1,2-c]isoxazole, 5-bromo-3a,4-dihydro-8-(methylthio)- (9CI) (CA INDEX NAME)



IT **293312-30-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of tricyclic aroylcyclohexanediones as herbicides)

RN 293312-30-8 CAPLUS

L29 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 3H-Indeno[1,2-c]isoxazole, 5-bromo-3a,4-dihydro-8-(methylsulfonyl)- (9CI) (CA INDEX NAME)

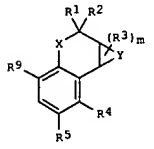


L29 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:666731 CAPLUS
DOCUMENT NUMBER: 133:237998
TITLE: Preparation of tricyclic benzoylpyrazoles as herbicides.
INVENTOR(S): Witschel, Matthias; Kudis, Steffen; Langemann, Klaus; Baumann, Ernst; Von Deyn, Wolfgang; Mayer, Guido; Misslitz, Ulf; Neidlein, Ulf; Otten, Martina; Westphalen, Karl-Otto; Walter, Helmut
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 168 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000055158 | A1 | 20000921 | WO 2000-EP2010 | 20000308 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2367672 | AA | 20000921 | CA 2000-2367672 | 20000308 |
| EP 1163240 | A1 | 20011219 | EP 2000-915171 | 20000308 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2002539211 | T2 | 20021119 | JP 2000-605587 | 20000308 |

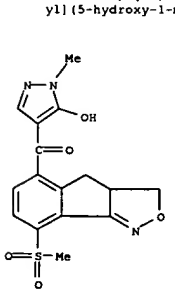
PRIORITY APPLN. INFO.: DE 1999-19911219 A 19990312
WO 2000-EP2010 W 20000308

OTHER SOURCE(S): MARPAT 133:237998
GI



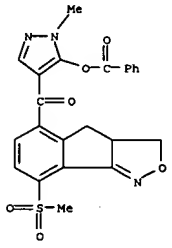
AB Title compds. [I; X = O, S, SO, SO2, CR6R7, NR8, bond; Y = atoms to form a saturated, partially saturated or unsatd. 5- or 6-membered heterocycle; R1, R2,

L29 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
R6, R7 = H, alkyl, haloalkyl, alkoxy, haloalkoxy; R3 = halo, alkyl, haloalkyl, alkoxy, haloalkoxy; R4 = H, NO2, halo, cyano, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl, haloalkylsulfonyl, (substituted) aminosulfonyl; R5 = H, alkyl, halo; m = 0, 1, 2; R8 = H, alkyl, haloalkyl, alkylcarbonyl, formyl, alkoxycarbonyl, haloalkoxycarbonyl, alkylsulfonyl, haloalkylsulfonyl; R9 = substituted pyrazole-4-ylcarbonyl, 5-oxopyrazolin-4-ylmethylides], were prepd. Thus, (5-hydroxy-1-methyl-1H-pyrazol-4-yl)(8-methylsulfonyl-3a,4-dihydro-3H-indeno[1,2-c]isoxazol-5-yl)methanone (prepn. given) in THF was treated with Et3N and PhCOCl in THF followed by stirring overnight to give 31% (5-phenylcarbonyloxy-1-methyl-1H-pyrazol-4-yl)(8-methylsulfonyl-3a,4-dihydro-3H-indeno[1,2-c]isoxazol-5-yl)methanone. The latter at 0.25-0.5 kg/ha showed very good postemergent herbicidal activity.
IT **293312-14-8P 293312-15-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tricyclic benzoylpyrazoles as herbicides)
RN 293312-14-8 CAPLUS
CN Methanone, [3a,4-dihydro-8-(methylsulfonyl)-3H-indeno[1,2-c]isoxazol-5-yl](5-hydroxy-1-methyl-1H-pyrazol-4-yl)- (9CI) (CA INDEX NAME)

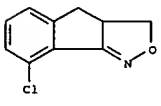


RN 293312-15-9 CAPLUS
CN Methanone, [5-(benzoyloxy)-1-methyl-1H-pyrazol-4-yl][3a,4-dihydro-8-(methylsulfonyl)-3H-indeno[1,2-c]isoxazol-5-yl]- (9CI) (CA INDEX NAME)

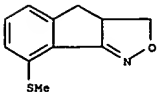
L29 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **293312-27-3P 293312-28-4P 293312-29-5P**
**293312-30-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tricyclic benzoylpyrazoles as herbicides)
RN 293312-27-3 CAPLUS
CN 3H-Indeno[1,2-c]isoxazole, 8-chloro-3a,4-dihydro- (9CI) (CA INDEX NAME)

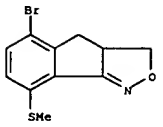


RN 293312-28-4 CAPLUS
CN 3H-Indeno[1,2-c]isoxazole, 3a,4-dihydro-8-(methylthio)- (9CI) (CA INDEX NAME)

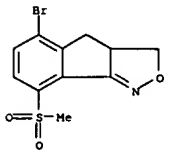


RN 293312-29-5 CAPLUS
CN 3H-Indeno[1,2-c]isoxazole, 5-bromo-3a,4-dihydro-8-(methylthio)- (9CI) (CA INDEX NAME)

L29 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

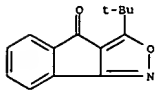


RN 293312-30-8 CAPLUS
CN 3H-Indeno[1,2-c]isoxazole, 5-bromo-3a,4-dihydro-8-(methylsulfonyl)- (9CI) (CA INDEX NAME)

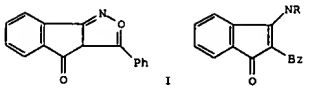


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

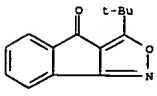
L29 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:34042 CAPLUS
DOCUMENT NUMBER: 100:34042
TITLE: Structure elucidation using signal intensity effects in carbon-13 nuclear magnetic resonance
AUTHOR(S): Shapiro, M. J.; Kolpak, M. X.; Lemke, T. L. L.
CORPORATE SOURCE: Dep. Pharm. Med. Chem., Sandoz Inc., East Hanover, NJ,
07936, USA
SOURCE: Journal of Organic Chemistry (1984), 49(1), 187-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Methods for structure elucidation utilizing the perturbation of non-protonated carbon signal intensities are presented. The effects of exchange deuteration and the techniques of difference heteronuclear NOE are described.
IT 82501-28-8
RL: PRP (Properties)
(structure elucidation of, proton-decoupled carbon-13 NMR and difference heteronuclear NOE in relation to)
RN 82501-28-8 CAPLUS
CN 4H-Indeno[1,2-c]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



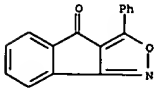
L29 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:612439 CAPLUS
DOCUMENT NUMBER: 99:212439
TITLE: Ring opening reactions of indeno[1,2-c]isoxazolones
AUTHOR(S): Lemke, Thomas L.; Sawhney, Kailash N.
CORPORATE SOURCE: Coll. Pharm., Univ. Houston, Houston, TX, 77004, USA
SOURCE: Journal of Heterocyclic Chemistry (1983), 20(4), 899-901
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:212439
GI



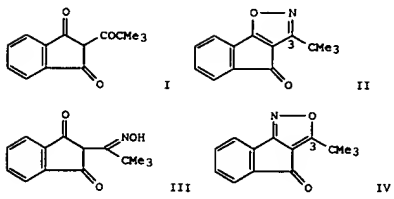
AB Nucleophilic attack of 8-substituted indeno[1,2-c]isoxazol-7-ones and 3-phenylindeno[1,2-c]isoxazol-4-one by Me2SO or PPh3 results in cleavage of the N-O bond of the isoxazole ring leading to the formation of sulfoximides and phosphazenes. Thus, treating indenoisoxazolone I with Me2SO and PPh3 gave II (R = NSOMe2, NPPh3), resp.
IT 82501-28-8 87885-96-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring cleavage of)
RN 82501-28-8 CAPLUS
CN 4H-Indeno[1,2-c]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



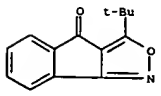
RN 87885-96-9 CAPLUS
CN 4H-Indeno[1,2-c]isoxazol-4-one, 3-phenyl- (9CI) (CA INDEX NAME)



L29 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:71358 CAPLUS
DOCUMENT NUMBER: 98:71358
TITLE: The utilization of chemical shift and spin-lattice (T1) relaxation time data for the discrimination of isomeric indenoisoxazoles
AUTHOR(S): Womack, Charles H.; Gampe, Robert T., Jr.; Lemke, B. Kaye; Sawhney, Kailash N.; Lemke, Thomas L.; Martin, Gary E.
CORPORATE SOURCE: Coll. Pharm., Univ. Houston, Houston, TX, 77004, USA
SOURCE: Journal of Heterocyclic Chemistry (1982), 19(5), 1105-7
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

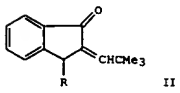


AB Treatment of I with NH2OH under acidic conditions gave II. Similar reaction of I under neutral or basic conditions gave III which was cyclized to IV. 13C NMR was used to differentiate II from IV based on assignments made using T1 relaxation as a guide; in the case of II the C(3) resonance is mediated by both the 14N-13C dipolar mechanism and by the nine Me3C protons while the C(3) of IV is relaxed solely by the Me3C protons. II and IV are also chemical differentiable.
IT 82501-28-8
RL: PRP (Properties)
(carbon-13 NMR and spin-lattice relaxation of)
RN 82501-28-8 CAPLUS
CN 4H-Indeno[1,2-c]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



L29 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:455721 CAPLUS
DOCUMENT NUMBER: 97:55721
TITLE: Synthesis and chemical reactivity of indenoisoxazoles
AUTHOR(S): Lemke, Thomas L.; Sawhney, Kailash N.; Lemke, B. Kaye
CORPORATE SOURCE: Coll. Pharm., Univ. Houston, Houston, TX, 77004, USA
SOURCE: Journal of Heterocyclic Chemistry (1982), 19(2), 363-8
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:55721
GI

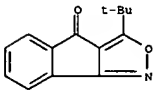


II

AB Treatment of 2-pivaloyl-1,3-indandione with NH2OH under acidic conditions, results in formation of 8-tert-butylindeno[1,2-c]isoxazol-7-one (I) while at neutral or basic pH 3-tert-butylindeno[1,2-c]isoxazol-4-one was obtained. The latter compound was readily reduced to amine with N2H4 or H-Pt. The amine, although quite unreactive, was converted to 3-tert-butylindeno[1,2-c]pyrazol-4-one with N2H4 or reduced to II (R = H, OH) with Na-NH3-Me3COH. Surprisingly, the amine obtained from I gave II (R = H) from a Na-NH3 reduction Spectral evidence for each of the structures is discussed.

IT **82501-28-8P 82501-29-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

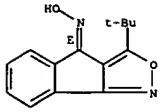
RN 82501-28-8 CAPLUS
CN 4H-Indeno[1,2-c]isoxazol-4-one, 3-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RN 82501-29-9 CAPLUS
CN 4H-Indeno[1,2-c]isoxazol-4-one, 3-(1,1-dimethylethyl)-, oxime, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





=> log y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 277.99 | 1129.75 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -40.88 | -40.88 |

STN INTERNATIONAL LOGOFF AT 06:19:32 ON 21 NOV 2005